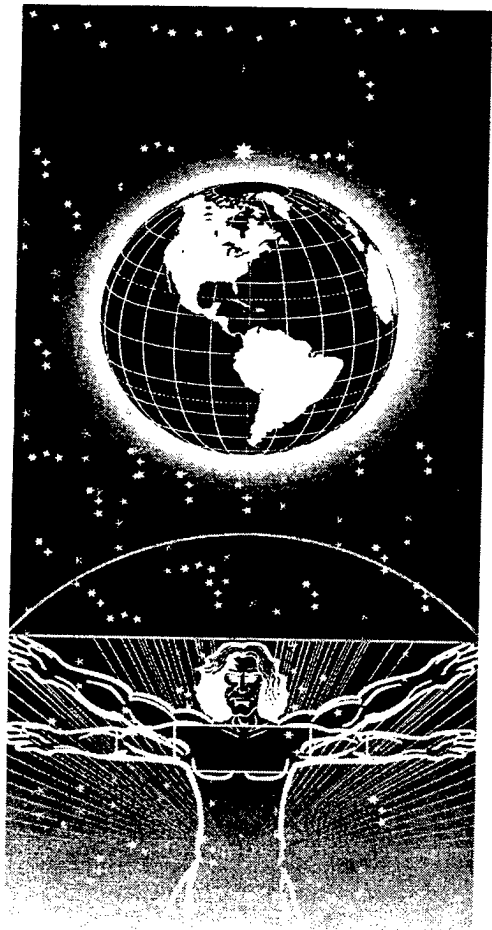AL/EQ-TP-1997-0021

UNITED STATES AIR FORCE
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Funnel-and-Gate Design Method

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The 'funnel/gate' system is a developing technology for passive groundwater plume management and treatment. This technology uses impermeable funnel walls to force polluted groundwater through a highly permeable zone of reactive porous media, the 'gate', where contaminants are degraded by biotic or abiotic heterogeneous reactions. The purpose of this study is to first develop and demonstrate analytical flow and fate/transport models for funnel/gate systems, and second, to develop and demonstrate a minimum cost design model. A series of equations which constitute an analytical, multi-contaminant, degradation and transport model have been developed. From an existing analytical hydraulic model for funnel/gate systems developed by Christensen and Hatfield (1994), an iterative design algorithm was developed for dimensioning a funnel/gate system. A funnel/gate cost estimation model with a Lagrangian optimization model was also developed to identify minimum cost designs subject to four constraints: one that defines the desired hydraulic retention time in the gate, one that defines the funnel wall length in terms of other system dimensions, and two that serve as hydraulic constraints. Finally a computer program was developed to demonstrate the theory that was developed. The Funnel/Gate Design Model (FGDM) software is a FORTRAN program developed to ascertain feasible dimensions of funnel/gate systems and also identify the lowest cost design.

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PREFACE

The work described in this report covers the contract period of July 1995 through April 1996. This work was performed by the Univeristy of Florida, Gainesville, Florida, under a consulting agreement with Applied Research Associates (ARA), Inc., Contract F08635-93-C-0020, Subtask 8.03, U.S. Air Force AL/EWQ, Barnes Drive, Suite 2, Tyndall Air Force Base, Florida. During the course of this study, there were two project officers, Major Mark H. Smith and Captain Jeff Stinson, BSC. This work was performed under the technical guidance of Mr. Robert E. Walker, ARA. This report was written by Kirk Hatfield of the University of Florida and edited by Mr. Walker.

EXECUTIVE SUMMARY

The 'funnel/gate' system is a developing technology for passive groundwater plume management and treatment. This technology uses impermeable funnel walls to force polluted groundwater through a highly permeable zone of reactive porous media, the 'gate,' where contaminants are degraded by biotic or abiotic heterogeneous reactions. The purpose of this study is to first develop and demonstrate analytical flow and fate/transport models for funnel/gate systems, and second, to develop and demonstrate a minimum cost design model.

A series of equations which constitutes an analytical, multicontaminant, degradation and transport model has been developed. This model can be applied in iterative manner to determine the critical hydraulic residence time, T, required to achieve specified concentrations of contaminants within a gate (e.g., to be certain that the water quality at the gate exit meets a specified water quality standard i.e., 1 µg/l vinyl chloride).

From an existing analytical hydraulic model for funnel/gate systems developed by Christensen and Hatfield (1994), an iterative design algorithm was developed for making a funnel/gate system dimensional. The design algorithm requires the following site and system data to execute:

a)   the critical hydraulic residence time in the gate;

b)   the transverse width of groundwater flow to be intercepted within the funnel, B;

c)   the saturated thickness of the phreatic aquifer, ϕ_1, at the entrance of the funnel;

d)   the groundwater flow through the area defined by width B and flow thickness, ϕ_1;

e)   the aquifer hydraulic conductivity;

f)   the porosity of the reactive porous media within the gate; and

g)   the hydraulic conductivity of the porous media within the gate.

Results of two FRAC-3D numerical validation studies are also presented. Thus, results of the numerical validation suggest the funnel/gate design model could be used to predimension

a system; however, subsequent numerical simulations should be conducted to verify the hydraulics of the design.

A funnel/gate cost estimation model was also developed to identify minimum cost designs subject to four constraints: one that defines the desired hydraulic retention time in the gate, one that defines the funnel wall length in terms of other system dimensions, and two that serve as hydraulic constraints. Costs considered in the model include land costs, costs per unit length of funnel walls, costs per unit length of gate, costs per unit width of gate, and costs associated with the reactive medium used in the gate. As a result of recasting into a Lagrangian optimization model, the optimization problem was reduced to that of solving a system of nine nonlinear equations with nine unknowns. Recommendations were given as to how the nine equations could be solved.

Finally a computer program was developed to demonstrate the theory that was developed. The Funnel/Gate Design Model (FGDM) software is a FORTRAN program developed to ascertain feasible dimensions of funnel-and-gate systems and also identify the lowest cost design.

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INTRODUCTION

OBJECTIVE

The purpose of this study is to first develop and demonstrate analytical flow and fate/transport models for funnel/gate systems, and second, to develop and demonstrate a minimum cost design model.

BACKGROUND

The 'funnel/gate' system is a developing technology for passive groundwater plume management and treatment. This technology uses impermeable funnel walls to force polluted groundwater through a highly permeable zone of reactive porous media, the "gate," where contaminants are degraded by biotic or abiotic heterogeneous reactions.

Figure 1 illustrates a plan view of a funnel/gate system of symmetrical configuration. This system contains matching sets of funnel walls. The first set of funnel walls serves to intercept the plume and direct polluted groundwater into the gate; whereas, the second set functions to disperse the decontaminated groundwater as it exits the gate. The funnel walls may be slurry walls or sheet piles keyed into an underlying aquitard.

As suggested above, groundwater decontamination occurs inside the gate. Here, dissolved contaminant removal is achieved through heterogeneous degradation reactions on the gate porous media alone or through the action of biotic/abiotic processes supported in the gate (i.e., bioremediation or sparging).

To design a funnel/gate system it is essential to first estimate a "critical hydraulic residence time" for groundwater flowing through the gate. The duration of this time is chosen to achieve "adequate contact time" between the intercepted groundwater and the reactive gate porous media. In this report, adequate contact time refers to the minimum time needed to bring polluted groundwater in contact with the reactive gate porous media such that dissolved contaminants are reduced to desired levels; that is, to be certain water quality at the gate exit

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Direction of Groundwater Flow

X = 0

PLUME

GATE

FUNNEL WALLS
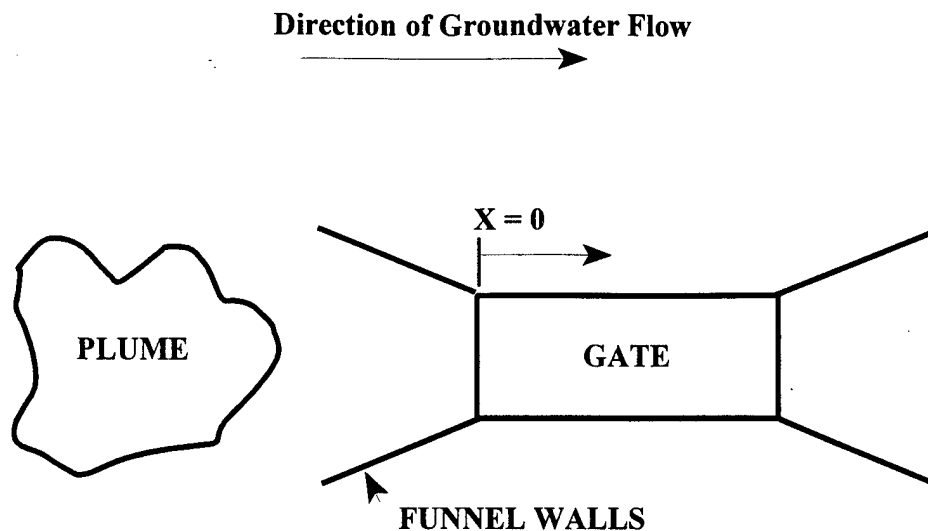
Figure 1.   Conceptual Plan View of a Funnel/Gate System.

meets specified water quality goals (i.e., system performance standards or drinking water standards i.e., 1 µg/l vinyl chloride).

Several pollutants may be targeted for destruction in a funnel/gate. For each target contaminant, the adequate contact time is determined. For each contaminant, this is achieved using the observed maximum plume concentrations, the expected degradation rate coefficient in the gate, and the water quality goal applied to water leaving the gate. For a plume comprised of several target contaminants (i.e., PCE and TCE), a critical hydraulic residence time must be determined. Here, the critical hydraulic residence time equals the longest adequate contact time in the gate which ensures all target contaminants meet desired water quality goals at the gate exit.

Once the critical hydraulic residence time in gate is known, the funnel and gate can be dimensioned following the approach of Christensen and Hatfield (1994), and using information on:

a) the transverse width of groundwater flow to be intercepted within the funnel, this is usually taken to be the width of the plume;

b) the saturated thickness of the phreatic aquifer at the entrance of the funnel;

c) the hydraulic gradient of groundwater flow;

d) the aquifer permeability;

e) the porosity of the reactive porous media within the gate; and

f) the permeability of the porous media in the gate.

SCOPE

This report describes hydraulic and contaminant fate and transport theories applicable to designing funnel/gate systems. In addition, the report describes a software package, Funnel/Gate Design Model (FGDM), which was developed to identify minimum cost design configurations. In Section 2, contaminant fate and transport theories are presented as they apply to dissolved pollutant degradation inside a reactive gate. Section 3 reviews the hydraulics of funnel/gate systems as previously presented by Christensen and Hatfield (1994). In Section 4, a design model for minimizing funnel/gate system costs is developed. Section 5 reviews the FGDM software and results from an example problem. Finally, Section 6 lists the FGDM FORTRAN code with example input and output files.

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SECTION II

CONTAMINANT FATE AND TRANSPORT THEORY

The first objective of this chapter is to present contaminant fate and transport theories pertinent to funnel/gate systems. A second but equally important objective is to develop an analytical contaminant degradation and transport model for the gate.

THEORY

Contaminant fate and transport has received considerable attention in groundwater systems. For funnel/gate systems, research has focused on the fate and transport of groundwater contaminants targeted for destruction inside the gate. Much of this research has examined reductive dehalogenation of chlorinated alkenes and alkanes using zero valent iron (Gillham and O'Hannesin, 1994; Schreier and Reinhard, 1994; Warren, Arnold, Bishop, Lindholm, and Betterton, 1995; and Burris, Campbell, and Manoranjan, 1995). Gillham and O'Hannesin (1994) and Burris[1] have looked at the degradation of tetrachloroethylene (PCE), trichloroethylene (TCE), dichloroethylene (DCE), vinyl chloride and other halogenated aliphatics using zero valent iron. A fraction of this degradation occurs within a sequential reductive dehalogenation process that transforms PCE to TCE, TCE to DCE, and DCE to vinyl chloride (Gillham and O'Hannesin, 1995; and Burris[1]). In addition to this sequence of reactions, Gillham and O'Hannesin (1995) and Burris[1] have indicated evidence of competing processes whereby PCE, TCE, DCE are transformed to other products such as PCE degradation to dichloroacetylene, TCE to chloroacetylene, and DCE degradation to acetylene. Figure 2 summarizes these reactions. Parameters λ_{1A}, λ_{2A}, λ_{2B}, etc., appearing in the figure correspond to degradation rate coefficients.

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[1]Burris, D.R., Personal Communication, Armstrong Laboratory, AL/EQC, 139 Barnes Drive, Tyndall AFB, FL 32403, 1995.
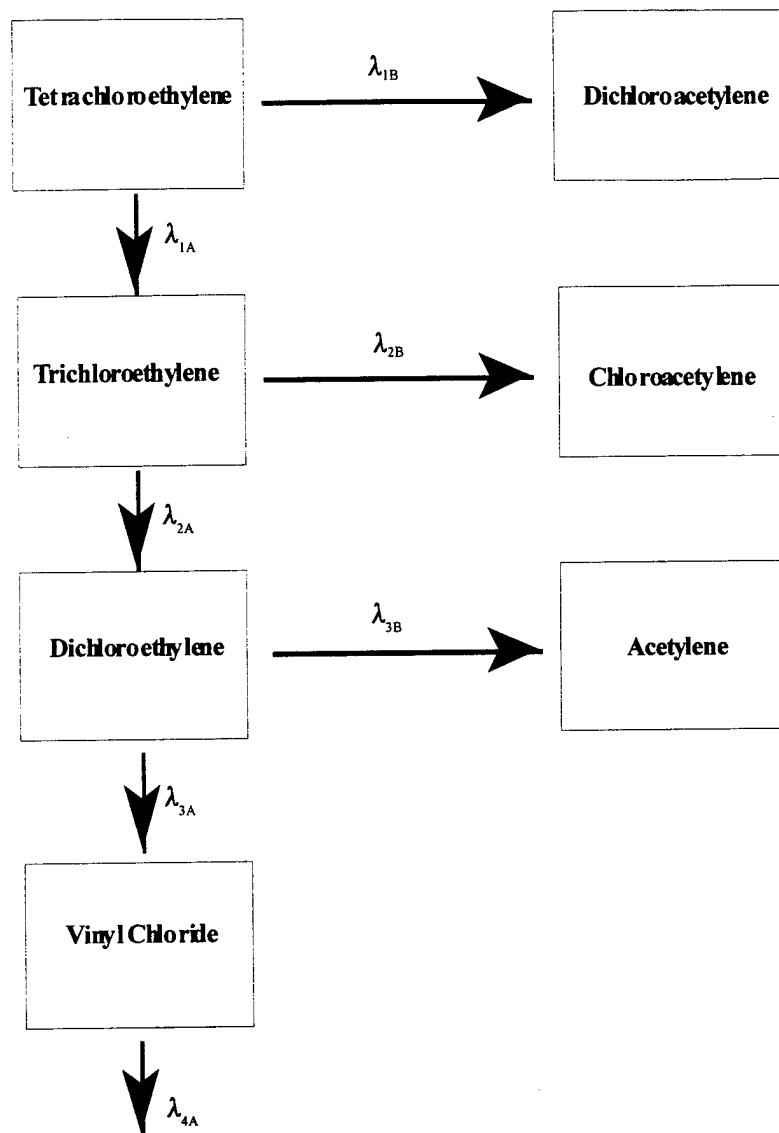
Figure 2. Conceptual Model of Reactions Involving Tetrachloroethylene, Trichloroethylene, Dichloroethylene, and Vinyl Chloride.

To develop a model describing the contaminant fate and transport inside the gate of a funnel/gate system, it is necessary to adopt a conceptual model of the reaction configuration. That is, a conceptual model descriptive of the reactions encountered with a dissolved contaminant inside the gate. Following the reaction configuration illustrated in Figure 2, a conceptual model was developed to generally describe not only the sequential degradation of chlorinated alkenes but also other contaminants (i.e., nitrate). Thus, Figure 3 shows contaminant C_1 degrading to C_2, then C_2 to C_3, then C_3 to C_4, and finally the degradation of C_4. If it is assumed that C_1, C_2, C_3, and C_4 respectively correspond to contaminants PCE, TCE, DCE, and vinyl chloride, then the reaction conceptual model, as illustrated in Figure 3, is sufficient to describe the degradation of these contaminants in the gate.

Inside the gate, advection (as opposed to dispersion) is the dominant transport mechanism. Using Figure 3 and assuming the gate flow field to be one-dimensional, governing steady-state fate and transport equations can be written in terms of contaminant concentration variables C_1, C_2, C_3, and C_4. Thus,

$$v\frac{\partial C_1}{\partial X} = -\lambda_{1A}C_1 - \lambda_{1B}C_1 \tag{1}$$

$$v\frac{\partial C_2}{\partial X} = -\lambda_{2A}C_2 - \lambda_{2B}C_2 + \lambda_{1A}C_1 \tag{2}$$

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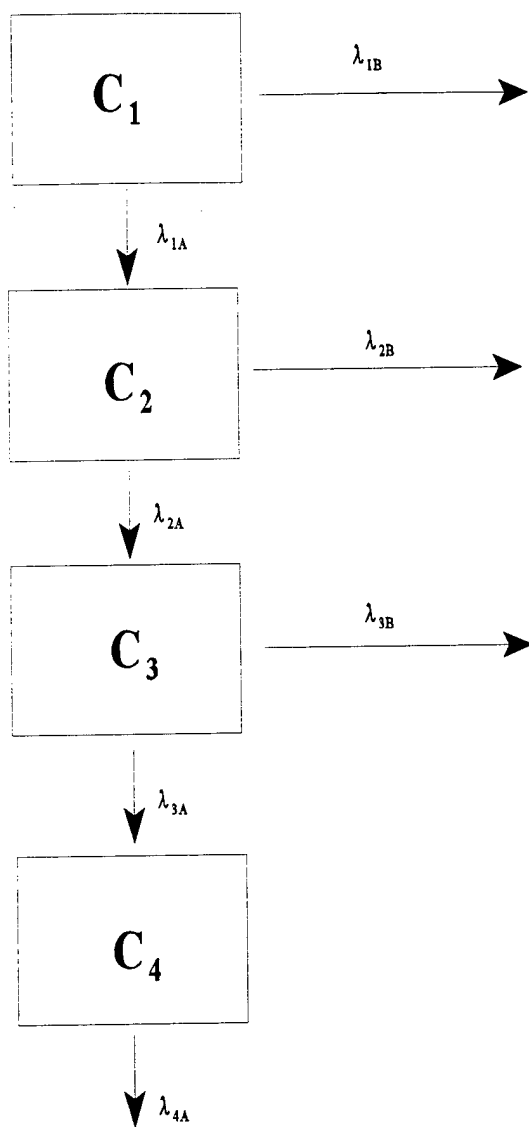
Figure 3.   General Conceptual Model of the Reaction Configuration Inside the Gate of
a Funnel/Gate System.

$$v \frac{\partial C_3}{\partial X} = - \lambda_{3A} C_3 - \lambda_{3B} C_3 + \lambda_{2A} C_2 \qquad (3)$$

$$v \frac{\partial C_4}{\partial X} = - \lambda_{4A} C_4 + \lambda_{3A} C_3 \qquad (4)$$

where v = unidirectional pore water velocity for groundwater flowing through the gate; X = the longitudinal distance measured from the gate entrance that runs parallel to the direction of groundwater flow through the gate (see Figure 1); and λ_{1A}, λ_{1B}, λ_{2A}, λ_{2B}, λ_{3A}, λ_{3B}, and λ_{4A}, = first order degradation coefficients as illustrated in Figure 3.

Equations (1) through (4) are simple advective transport equations which assume unidirectional, uniform, and constant pore velocities throughout the gate. These equations assume contaminant concentrations are invariant along transverse Y and Z directions; consequently, they are limited to describing steady-state concentration profiles of C_1, C_2, C_3, and C_4 in the gate and along the X axis alone.

ANALYTICAL MULTI-CONTAMINANT DEGRADATION AND TRANSPORT MODEL

Analytical solutions to Equations (1) through (4) can be obtained under the assumption that influent concentrations are constant and known for C_1, C_2, C_3, and C_4 at the gate entrance ($X = 0$). This is equivalent to assuming boundary conditions that specify concentrations variables C_1, C_2, C_3, and C_4 as having values of C_{10}, C_{20}, C_{30}, and C_{40} respectively at the $X = 0$. In the field, contaminant concentrations are never constant at the gate entrance, but vary with time as a plume is intercepted. As a result, it will be necessary in practice to let C_{10}, C_{20}, C_{30}, and C_{40} equal maximum plume concentrations of four contaminants identified in a plume and targeted for destruction inside the gate. Under this approach, a critical hydraulic residence is found which is suitable for treating maximum observed pollutant concentrations.

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Using the above boundary assumption, that $C_1 (X = 0) = C_{10}$, the solution to Equation (1) is:

$$C_1(T) = C_{10} \cdot EXP[- jT] \tag{5}$$

where

$$j = \lambda_{1A} + \lambda_{1B} \tag{6}$$

and T = the hydraulic residence time as defined by Eq. (7) below:

$$T = \frac{X}{v} \tag{7}$$

Equation (5) describes the steady-state concentration profile of contaminant C_1 throughout the length of the gate.

Using Equation (5) and the boundary condition defining $C_2 (X = 0) = C_{20}$, the solution to Equation (2) is:

$$C_2(T) = C_{20} \cdot EXP[- gT] + \frac{KC_{10}}{(g - j)}[EXP[- jT] - EXP[- gT]] \tag{8}$$

where

$$g = \lambda_{2A} + \lambda_{2B} \tag{9}$$

and

$$K = \lambda_{1A} \tag{10}$$

Equation (8) describes the steady-state concentration profile of contaminant C_2 throughout the length of the gate as a consequence of C_2 degradation and of C_2 production from C_1 degradation.

Again, Equation (3) is solved similarly, using Equation (8) and the above stated boundary condition of $C_3 (X = 0) = C_{30}$. Thus,

$$C_3(T) = A \cdot EXP[-mT] + E \cdot EXP[-jT] + D \cdot EXP[-gT] \qquad (11)$$

Where

$$A = C_{30} - \frac{fC_{20}}{(g-j)(m-j)} + \frac{fKC_{10}}{(g-j)(m-g)}$$

$$+ \frac{fKC_{10}}{(g-j)(m-g)} \qquad (12)$$

$$E = \frac{fKC_{10}}{(g-j)(m-j)} \qquad (13)$$

$$D = \frac{fC_{20}}{(m-g)} - \frac{fKC_{10}}{(g-j)(m-g)} \qquad (14)$$

$$f = \lambda_{2A} \qquad (15)$$

and

$$m = \lambda_{3A} + \lambda_{3B} \qquad (16)$$

Thus, Equation (11) describes the steady-state concentration profile of contaminant C_3 throughout the length of the gate as both a consequence of C_3 degradation to C_4 and of C_3 production from C_2 degradation.

Finally, substituting Equation (11) into Equation (4) and using the above stated boundary condition of C_4 $(X = 0) = C_{40}$, the following function is obtained for C_4 concentration distributions inside the gate:

$$C_4(T) = G \cdot EXP[-HT] + \frac{PA}{(H - m)} EXP[-mT]$$

$$+ \frac{PE}{(H - j)} EXP[-jT] + \frac{PD}{(H - g)} EXP[-gT] \qquad (17)$$

where

$$G = C_{40} - \frac{PA}{(H - m)} - \frac{PE}{(H - j)} - \frac{PD}{(H - g)} \qquad (18)$$

$$H = \lambda_{4A} \qquad (19)$$

and

$$P = \lambda_{3A} \qquad (20)$$

Equation (17) describes steady-state C_4 concentration profiles that reflect degradation and C_4 production from C_3 degradation.

SUMMARY

Equations (5), (8), (11), and (17) constitute an analytical, multi-contaminant, degradation and transport model. This model can be applied in iterative manner to determine the critical hydraulic residence time, T, required to achieve specified concentrations of contaminants C_1, C_2, C_3, and C_4 within a gate (e.g., to be certain that the water quality at the gate exit meets a specified

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water quality standard such as 1 μg/l vinyl chloride). To use this transport model, the following data are needed:

a)   degradation rate coefficients for all reactions depicted in Figure 3;

b)   specified water quality goals or system performance standards for C_1, C_2, C_3, and C4 (e.g., primary drinking water standards for PCE, TCE, DCE, and vinyl chloride); and

c)   the concentration of each contaminant at the entrance of the gate, C_{10}, C_{20}, C_{30}, and C_{40}. Once the critical hydraulic residence time is known, the hydraulic model can be used to dimension the system.

SECTION III

FUNNEL/GATE HYDRAULICS

This Section seeks to fulfill two objectives. The first is to review elements of an existing analytical hydraulic model for funnel/gate systems that was developed by Christensen and Hatfield (1994). The second objective is to compare analytical model predictions of funnel/gate system performance to those given by a complex numerical model, FRAC-3D.

THEORY

Christensen and Hatfield (1994) presented a model describing the steady-state hydraulics of a funnel/gate system. Model development was predicated on the symmetrical system configuration illustrated in Figure 4. This figure presents a conceptual plan view of a funnel/gate system about to capture a plume of width B_o. In addition, this figure shows groundwater, of flow width less-than-or-equal-to 'B,' being intercepted from an undisturbed flow field by an upstream funnel of entrance width B, and projected wall length, L. As a result of gravity, groundwater is forced through a gate of width, b, and length, ℓ. The hydraulic residence time inside the gate is T. As this groundwater exits the gate, flow diverges in a downstream funnel identical to the upstream funnel and is returned to the undisturbed flow field.

Christensen and Hatfield (1994) characterized groundwater flow up gradient, down gradient, and inside the funnel/gate by dividing the overall flow field into five zones (See Figure 5). Zones 1 and 5 respectively correspond to up gradient and down gradient undisturbed groundwater flow fields. Zone 2 is a converging flow zone created inside the upstream funnel; whereas, Zone 4 encompasses a region of divergent flow within the downstream funnel. Finally, there is Zone 3, inside the gate, where flow is assumed one-dimensional and horizontal.

As stated above, Zones 1 and 5 reflect undisturbed flow fields; however, in Zones 2, 3, and 4 there are changes in groundwater potential caused by a funnel/gate system that must be estimated. Christensen and Hatfield (1994) developed their hydraulic model treating the aquifer as an isotropic and homogeneous medium underlain by a horizontal aquiclude. In addition, they assumed the capillary fringe was minor, and that groundwater flow was undirectional, horizontal,

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ZONE 1   ZONE 2   ZONE 3   ZONE 4   ZONE 5

FUNNEL WALLS

B_0

B

X_2

$X_2 = 0$

$X_3 = 0$

GATE

X_4

$X_4 = 0$

b

B

L ℓ L
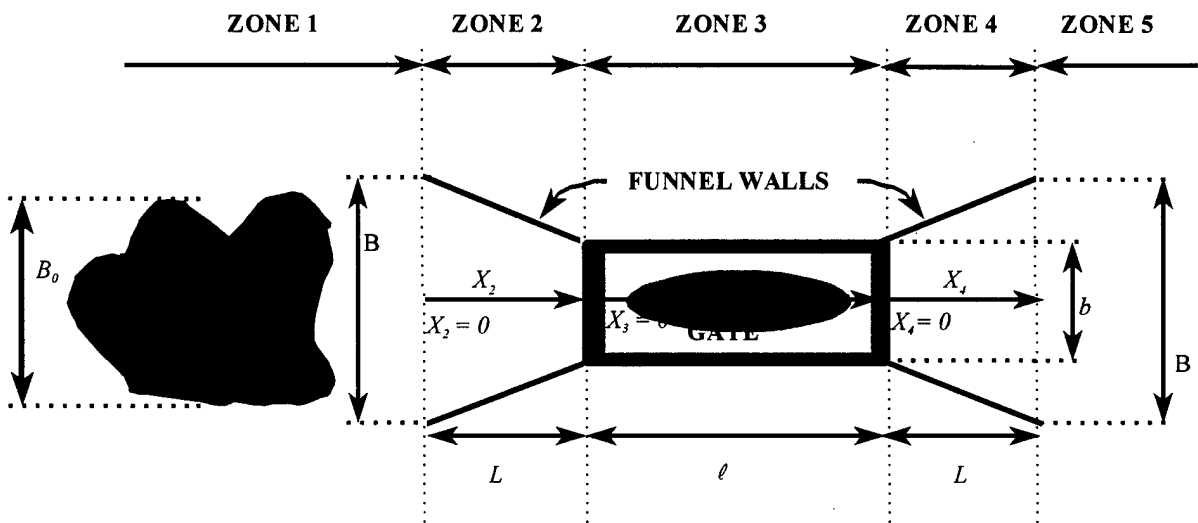
Figure 4.   Plan View of Symmetrical Funnel/Gate System Defining Geometry of Flow Boundaries.

and unconfined. From these assumptions, they derived the following functions which characterize groundwater potentials inside zones 2, 3, and 4, respectively:

$$\phi_2(X_2) = \left[\phi_1^2 + \frac{2QL}{k(B-b)} \ln\left(1 - \left[1 - \frac{b}{B} \right]^{\frac{X_2}{L}} \right) \right]^{\frac{1}{2}} \tag{21}$$

$$\phi_3(X_3) = \left[\phi_1^2 + \frac{2QL}{k(B-b)} \ln\frac{b}{B} - \frac{2QX_3}{k_o b} \right]^{\frac{1}{2}} \tag{22}$$

$$\phi_4(X_4) = \left[\phi_1^2 + \frac{2QL}{k(B-b)} \ln\frac{b}{B} - \frac{2Q\ell}{k_o b} - \frac{2QL}{k(B-b)} \ln\left(1 - \left[1 - \frac{b}{B} \right]^{\frac{X_4}{L}} \right) \right]^{\frac{1}{2}} \tag{23}$$

where ϕ_2, ϕ_3, and ϕ_4 = groundwater potentials in Zones 2, 3, and 4, respectively (these are also equivalent to aquifer saturated thicknesses in these zones if the zero datum is taken to be the top of the aquiclude); X_2, X_3, and X_4 = longitudinal distances from the upstream ends of Zones 2, 3, and 4, respectively (see Figure 4); ϕ_1 = the groundwater potential (or saturated aquifer thickness) at the entrance of the upstream funnel (where $X_2 = 0$ at the beginning of Zone 2); k = the hydraulic conductivity of aquifer; k_o = the hydraulic conductivity of the gate; and Q = the total rate of flow passing the width B in the undisturbed groundwater flow field.

The total rate of flow through the funnel/gate system, Q is estimated using the aquifer permeability, the width (B) of groundwater flow intercepted, the potential ϕ_1, at the funnel entrance, and the potential gradient, $d\phi/dx$, of the undisturbed flow field at $X_2 = 0$. Thus,

$$Q = B\phi_1 k \left(-\frac{d\phi}{dX} \right)\Big|_{X_2=0} \tag{24}$$

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The hydraulic residence time for the groundwater flowing through the gate, T, is given by:

$$T = \frac{\theta \, \ell \, b \, \phi_{gate}}{Q}$$
(25)

where θ = porosity of the gate and ϕ_{gate} = the average groundwater potential in the gate, which is taken here to equal the saturated thickness of the aquifer inside the gate. Design parameters Q and θ are usually known or specified, while T equals the critical hydraulic residence time identified by the transport model. Knowing that Q, θ, and T are constants, it follows from Equation (25) that the gate volume, $\ell b \phi_{gate}$, is also constant for an identified critical hydraulic residence time.

Generally, it may be assumed that the width of intercepted groundwater flow is less-than-or-equal-to B, the funnel width, and that $B \geq B_o$, the plume width. Under this assumption, Christensen and Hatfield (1994) found that the projected length of the funnel walls, L can be estimated from:

$$L = \frac{\ell}{2} \cdot \frac{\dfrac{k/k_o}{b/B} - 1}{\dfrac{\ln(b/B)}{1 - (b/B)} + 1}$$
(26)

ITERATIVE SOLUTION ALGORITHM TO DIMENSION A FUNNEL/GATE SYSTEM

To design a funnel/gate system, it is difficult to use Equations (25) and (26) directly. This is because gate length ℓ and potential ϕ_{gate} are generally unknown, and also because governing Equations (26), (25), and (21) or (22) must be satisfied simultaneously. As a result, L, ℓ, and ϕ_{gate} are estimated using an iterative approach.

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The design process begins assuming the funnel width B and the gate/funnel width ratio b/B are known; therefore, b is known. In practice, a suite of b/B ratios should be investigated. During the first step of the first iteration, the gate length is approximated using Equation (25) and substituting ϕ_1 as an initial approximation for ϕ_{gate}. Thus,

$$\ell \approx \frac{TQ}{\theta b \Phi_1} \qquad (27)$$

The next step uses the ℓ results of Equation (27) in Equation (26) to obtain an initial estimate of the projected funnel wall length, L. At the end of the first iteration, initial estimates of ℓ and L have been made.

During the first step of the second iteration, ϕ_{gate} is calculated using the function below:

$$\phi_{gate} = \left[\phi_1^2 + \frac{2QL}{k(B - b)} \ln \frac{b}{B} \right] \qquad (28)$$

Equation (28) can be derived either from Equation (21) assuming $X_2 = L$ or from Equation (22) assuming $X_3 = 0$. The second step uses the most recent estimate of ϕ_{gate} in Equation (25) to obtain an updated value for the gate length, ℓ. The third and final step of the second iteration uses the most recent estimate of ℓ in Equation (26) to obtain a new calculation of the projected funnel wall length, L.

Subsequent iterations repeat steps described under the second iteration; however during each step ℓ, L, and ϕ_{gate} estimates generated from the most recent iteration are used. The iterative process continues until changes in ℓ, L, and ϕ_{gate} values are less than 1 percent between iterations.

From the above presentation, it may be concluded that the hydraulic model can be used to dimension a funnel/gate system given the following information is available:

a)   the critical hydraulic residence time inside the gate;

b)   the transverse width of groundwater flow to be intercepted within the funnel, B,

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this is practically taken to be greater than the width of the plume;

c) the saturated thickness of the phreatic aquifer, ϕ_1, at the entrance of the funnel;

d) the groundwater flow through the area defined by width B and flow thickness, ϕ_1;

e) the aquifer hydraulic conductivity;

f) the porosity of the reactive porous media within the gate; and

g) the hydraulic conductivity of the porous media within the gate.

MODEL VALIDATION

To validate the funnel/gate hydraulic model, numerical simulations were performed to generate flow fields for several funnel/gate configurations dimensioned using the above analytical hydraulic model. The numerical simulations were conducted using FRAC-3D. The velocity fields generated from the numerical simulations were then used to create figures illustrating the groundwater flow streamlines. Figure 5 illustrates conceptually the orientation of a funnel/gate system in the numerical model. Shown is a wide funnel/gate system. The gate width, b, extends between funnel walls and is parallel to the X axis. The gate length, ℓ, extends parallel to the Y axis; thus, groundwater flows parallel to the Y axis. Finally, Figure 5 suggests that meters were used as the length dimension in the FRAC-3D simulations.

Before, the numerical model could be formulated, the analytical hydraulic model was used to configure specific funnel/gate dimensions, ℓ and L, using the following input data:

Site conditions:

$k = 4.32$ m/d

$\phi_1 = 5$ m

$d\phi/dx (X_2 = 0) = -0.005$

System design conditions:

$T = 11.0$ d

$\theta = 0.45$

$k_o = 43.2$ m/d

$B = 61$m

$b/B = 0.6$

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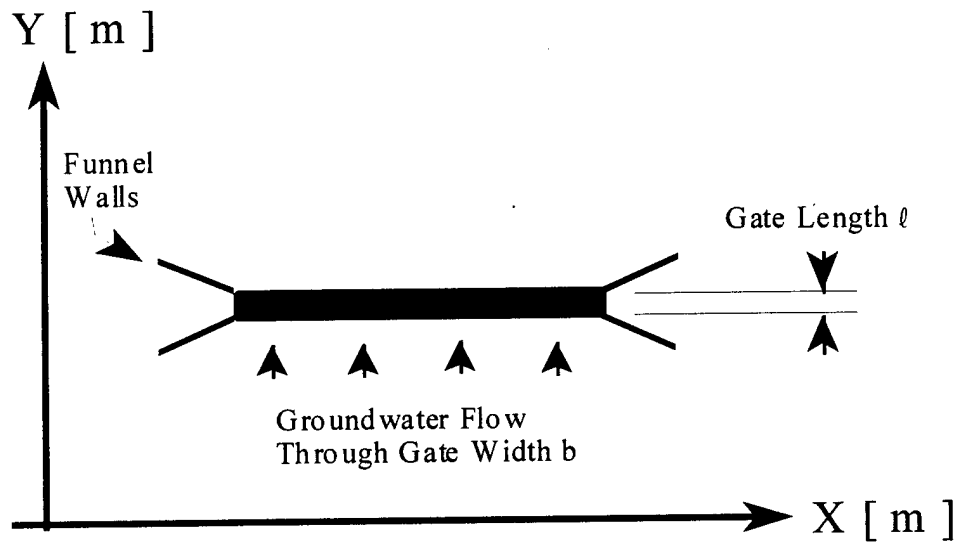
Figure 5.   Conceptual Orientation of the Funnel/Gate System in the FRAC-3D Flow Domain.

Feasible funnel/gate dimensions identified with the analytical model were:

$\ell = 0.9$ m

$L = 1.3$ m

$b = 36.6$ m

Keeping Figure 5 in mind, the groundwater flow simulation from FRAC-3D can be viewed in Figure 6. This figure is an illustration of simulated streamlines created in the groundwater flow field containing the above funnel/gate system design. The numerical values on both axes are distances expressed in meters. Groundwater is generally flowing parallel with the Y axis. The funnel walls are easily visible in Figure 6, and the gate width appears equal to
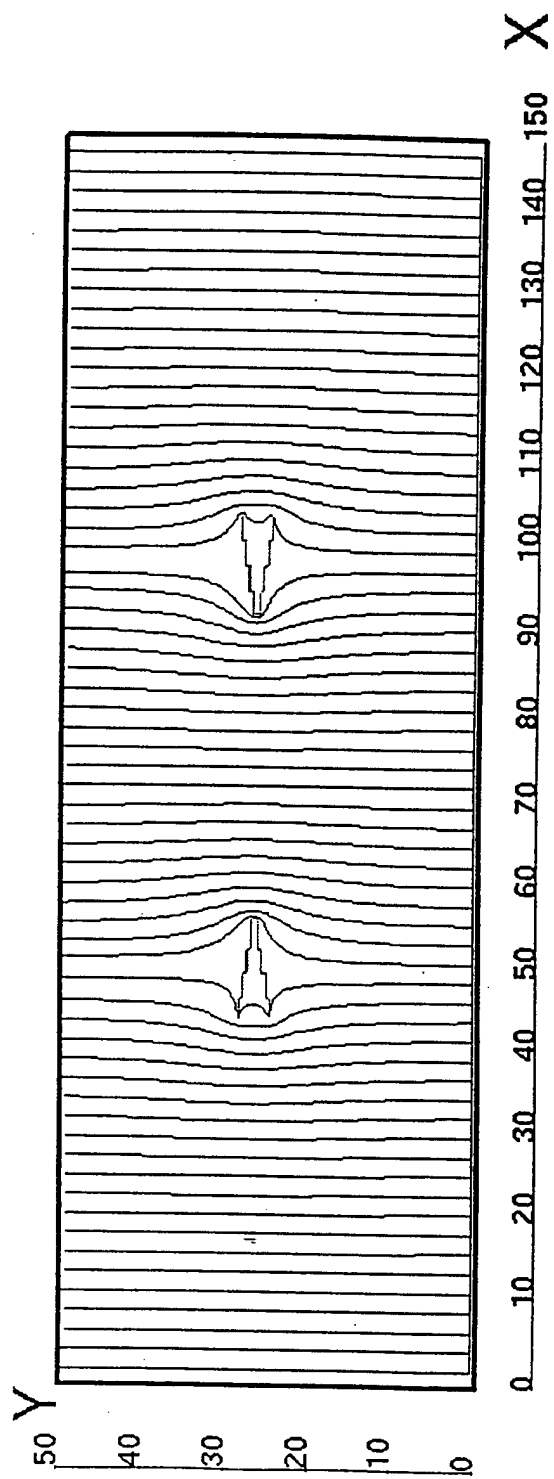
Figure 6. FRAC-3D Generated Streamlines for Funnel/Gate Validation Example 1.

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the above specified design width of 36.6 meters. The FRAC-3D simulation results show the resulting funnel/gate design intercepting close to 49 meters of flow width (as viewed from the streamlines); this represents 80 percent of the funnel design width of B = 61 meters. This suggests that the analytical model produced a funnel/gate design configuration that has an 80 percent capture efficiency. It also says the volummetric flow rate is 20 percent less than the design flow, Q; consequently, the numerically simulated hydraulic residence time in the gate will be longer than the critical hydraulic residence time. The extended residence time provides for additional contaminant degradation; thus, the system design is conservative in the regard that it will produce water with lower contaminant levels than the design quality. These results demonstrate that the analytical hydraulic model can identify feasible, albeit conservative, funnel/gate designs when appropriate information is provided.

In another validation effort, a second funnel/gate design was created using the same site and system conditions as described above, except that the width ratio b/B was increased to 0.7. The result of increasing the gate width, b, is that gate length, ℓ, will decrease such that the total gate volume remains unchanged; thus, the total volume of required reactive medium does not change. This happens as a consequence of Equation 25 and the specified critical hydraulic residence time of 11.0 days. Under the new width ratio, the analytical hydraulic model identified the following feasible funnel/gate dimensions:

$\ell = 0.15$ m

$L = .35$ m

$b = 42.7$ m

Figure 7 is an illustration of the groundwater flow streamlines simulated with FRAC-3D for a second funnel/gate design. Streamlines show this funnel/gate configuration intercepting a groundwater flow width of 52 meters or 85 percent of funnel design width. As expected, these results show that increasing the gate width b increases the capture efficiency of the system. Hence, a long interception trench or wide permeable wall is expected to be more efficient than a narrow gate; however, this says nothing about comparative costs of such configurations. These results suggest the funnel/gate design model could be used to pre-dimension a minimum cost system; however, subsequent numerical simulations should be conducted to verify the hydraulics

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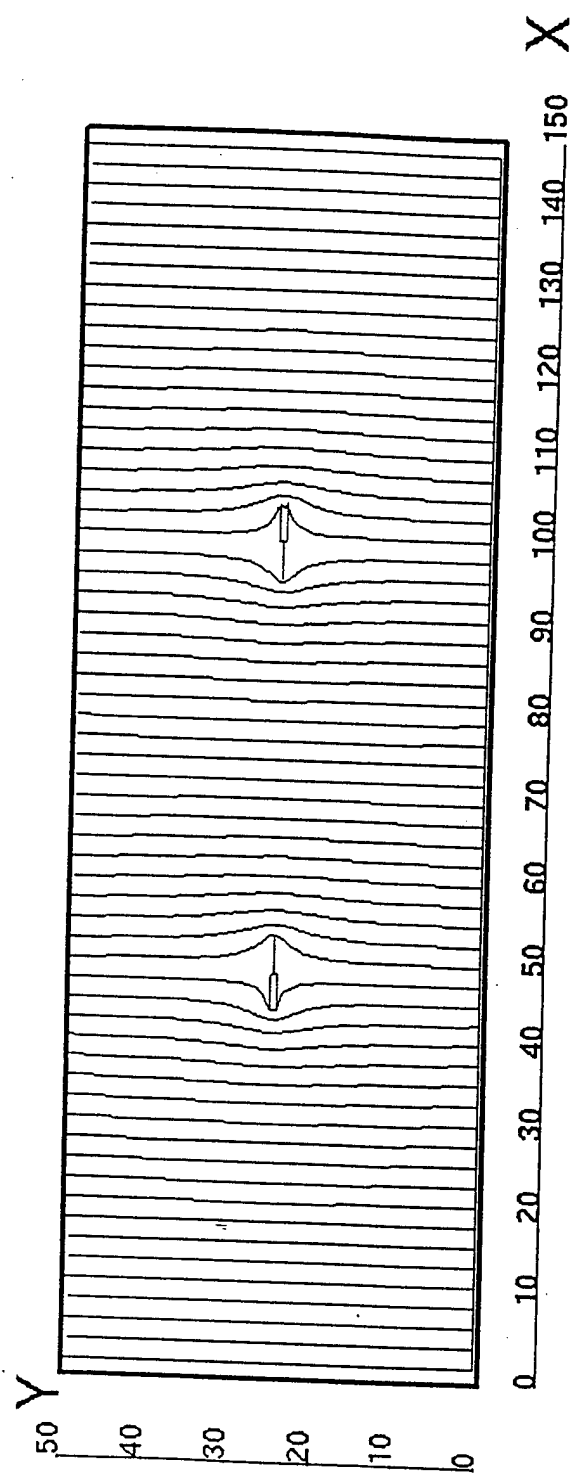
Figure 7. FRAC-3D Generated Streamlines for Funnel/Gate Validation Example 2.

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of the design. If these numerical simulations demonstrate that the proposed design is unable to intercept a plume of specified width, the funnel width, B, and/or the gate width, b, is increased to enhance capture.

SUMMARY

This section began with a brief review of an existing analytical hydraulic model for funnel/gate systems developed by Christensen and Hatfield (1994). From this an iterative design algorithm was developed for dimensioning a funnel/gate system. The design algorithm incorporates Equations (24) to (28) and requires the following site and system data to execute:

a) the critical hydraulic residence time in the gate;

b) the transverse width of groundwater flow to be intercepted within the funnel, B; this is practically taken to be greater than the width of the plume;

c) the saturated thickness of the phreatic aquifer, ϕ_1, at the entrance of the funnel;

d) the groundwater flow through the area defined by width B and flow thickness, ϕ_1;

e) the aquifer hydraulic conductivity;

f) the porosity of the reactive porous media within the gate; and

g) the hydraulic conductivity of the porous media within the gate.

In the last part of this section, results of two FRAC-3D numerical validation studies were presented. For the two funnel/gate systems examined, the numerical results showed the analytical design model produced system configurations which exhibited 80 to 85 percent capture efficiency. These efficiencies increase as the gate becomes wider. Thus, results of the numerical validation suggest the funnel/gate design model could be used to pre-dimension a system; however, subsequent numerical simulations should be conducted to verify the hydraulics of the design.

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SECTION IV

COST MINIMIZATION MODELING

The primary objective of this chapter is to develop a cost estimation model that will identify minimum cost funnel/gate designs. The secondary objective is to recast the general cost model into Lagrangian optimization formulation that is then amenable to solution.

COST OBJECTIVE FUNCTION

The total cost of funnel/gate systems can include at least the five components:

1) Construction/design costs per unit length of funnel wing walls;

2) Construction/design costs per unit length of gate;

3) Construction/design costs per unit Width of gate;

4) Land costs per unit area; and

5) Costs of reactive media installed in the gate.

Additional costs such as water quality monitoring before and after system installation are not presently considered.

Construction/design cost per unit length of funnel wing walls can be summarized as follows:

$$Total\ cost\ of\ 4\ funnel\ walls\ =\ 4E_1X_2 \tag{29}$$

where X_2 = the length of a single funnel wall; and E_1 = the cost per unit length of funnel wall. This unit cost is calculated as follows:

$$E_1\ =\ C_{sffw}\ d \tag{30}$$

in which d = depth of funnel walls (i.e. the depth to which slurry walls are constructed or the depth to which sheet piles are driven); and C_{sffw} = cost per unit area of sheet pile or slurry wall

used to construct the funnel walls. Clearly the cost parameter, C_{sffw} , varies with the total area of sheet pile used and the depth to which the sheet pile is driven. Table 1 presents C_{sffw} values for sheet pile where costs vary as a function of both total sheet pile area installed and pile depth.[2]

TABLE 1. C_{sffw} VALUES FOR SHEET PILE.

Sheet Pile Unit Costs C_{sffw} [Dollars]			
Sheet Pile Depth [m]	Sheet Pile Area [m^2]		
	< 465	465 - 860	> 1860
0 - 8	280	193	172
8 - 15	301	215	183
15 - 24	322	236	204

Construction/design costs per unit length of gate are quantified as follows:

$$\textit{Total cost of 2 longitudinal gate walls} = 2E_2 \ell \qquad (31)$$

where ℓ = the longitudinal gate length as defined in Section 3, and E_2 = the cost per unit length of longitudinal gate wall. E_2 estimated from:

$$E_2 = C_{sfgl} d \qquad (32)$$

in which C_{sfgl} = cost per unit area of sheet pile or slurry wall used to construct the longitudinal

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[2]Jowett, R., Personal Communication, Waterloo Educational Services, Inc., 2 Taggart Court, Unit 4, Guelph, Ontario N1H 6H8, 1996.

gate walls. Thus, E_2 may equal E_1 if gate and funnel walls are constructed using similar materials, i.e., $C_{sffw} = C_{sfgl}$.

Construction/design cost per unit width of the transverse gate wall can be summarized as follows:

$$Total \ cost \ of \ 2 \ transverse \ gate \ walls \ = \ 2E_3BX_1 \tag{33}$$

where $X_1 = b/B$, the dimensionless ratio of gate width to funnel width; B = the funnel wall entrance width as defined in Section 3; and E_3 = the cost per unit width of the transverse gate wall. This cost parameter is estimated from:

$$E_3 \ = \ C_{sfgw} \ d \tag{34}$$

in which C_{sfgw} = cost per unit area of sheet pile or trenching required to construct the transverse gate wall.

Land costs are estimated with:

$$Total \ Land \ Costs \ = \ E_{11} \ B \ (\ell \ + \ 2L) \tag{35}$$

where L = the projected length of the funnel walls as defined in Section 3; and E_{11} = land costs per unit area.

Finally, there is the cost of the reactive medium installed in the gate. This cost is essentially constant within a suite of alternative designs being examined for any single site. This is because the critical hydraulic residence time must be preserved between the different designs under investigation; it may be recalled from Section 2 that to allow the hydraulic residence time to vary between potential designs would produce different systems which are not comparable because each will achieve a different degree of contaminant degradation. In keeping with a constant critical hydraulic residence time, the gate volume becomes a known constant (so long as Q remains constant). The cost of the reactive gate material is estimated from:

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$$\text{Total cost of gate reactive media} = \frac{E_{12}QT}{\theta} \qquad (36)$$

in which Q = the volumetric flow through the gate as defined in Section 3, T = critical hydraulic residence time defined in Sections 2 and 3, and E_{12} = cost of reactive media per unit volume. The cost of iron is generally $1,690 - 1,760 m^{-3} (Jowett).[2]

Equations (29), (31), (33), (35), and (36) can be combined to obtain an overall cost objective function.

$$\text{Total funnel/gate costs} = 4E_1X_2 + 2E_2\ell + 2E_3BX_1 + E_{11}B(\ell + 2L) + E_{12}QT \qquad (37)$$

CONSTRAINTS

The minimum value of the cost objective function, Equation (37), is determined under a set of constraints which ensure that only feasible funnel/gate designs are identified (a feasible design being one that is correct both from hydraulic and from transport perspectives). In this study, four constraints were considered:

1) Constraint identifying feasible combinations of gate dimensions length, ℓ, width b, and saturated thickness, ϕ_{gate}, such that the critical hydraulic residence time is achieved inside the gate;

2) Constraint to identify feasible gate potentials (saturated thickness), ϕ_{gate}, that are consistent with the hydraulic model;

3) Constraint defining funnel walls lengths in terms of gate width, b, and projected funnel wall length, L;

4) Constraint to identify feasible combinations of projected funnel wall length, L, gate width, b, and gate length, ℓ, consistent with the hydraulic model.

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[2]Jowett, R., Personal Communication, Waterloo Educational Services, Inc., 2 Taggart Court, Unit 4, Guelph, Ontario, N1H 6H8, 1996.

The first constraint functions to ensure feasible combinations of gate dimensions width, b, length, ℓ, and saturated thickness, ϕ_{gate}, are identified to produce a saturated gate volume large enough to meet the critical hydraulic residence time, T. It may be recalled that the value of T is obtained from executing the transport model. It represents the longest "adequate contact time" in the gate which ensures all target contaminants meet desired water goals at the gate exit. Recalling Equation (25):

$$\frac{\theta \ell b \phi_{gate}}{Q} = T \tag{38}$$

or

$$BX_1 \ell X_5 - \frac{QT}{\theta} = 0 \tag{39}$$

where

$$X_5 = \phi_{gate} \tag{40}$$

Constraint Equation (39) ensures that the gate volume will be large enough to produce a hydraulic residence time equal to the specified critical hydraulic residence time.

The second constraint is required to ensure the cost model identifies feasible potentials (saturated thickness) in the gate that are consistent with the hydraulic model. This constraint is derived from Equation (28):

$$\phi_{gate} = \left[\phi_1^2 + \frac{2QL}{k(B - b)} \ln \frac{b}{B} \right]^{\frac{1}{2}} \tag{41}$$

Rearranging Equation (41) gives Equation (42), the final form of the second constraint on the gate potential:

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$$X_5^2(1 - X_1) - \phi_1^2(1 - X_1) - \frac{2QL}{kB}\ln[X_1] = 0. \tag{42}$$

The cost objective function, Equation (37), is defined in terms of variable X_2, the funnel wall length; consequently, the third constraint is required because it defines X_2 in terms of design variables, projected funnel wall length, L, and the dimesionless width ratio, X_1. Thus, from the funnel/gate system geometry the following constraint was derived:

$$X_2^2 - \frac{B^2}{4}(1 - 2X_1 + X_1^2) - L^2 = 0. \tag{43}$$

The fourth and final constraint is derived from Equation (26) rewritten below to include decision variable, X_1 :

$$L = \frac{\ell}{2} \cdot \frac{\dfrac{k/k_o}{X_1} - 1}{\dfrac{\ln(X_1)}{1 - (X_1)} + 1} \tag{44}$$

Equation (44) serves to limit the optimization model to examine only those combinations of projected funnel wall length, L, gate width, b, and gate length, ℓ, that will also meet hydraulic constraints defined by governing flow equations (i.e., continuity and momentum). A more convenient form for Equation (44) is:

$$2X_5(X_1\ln[X_1] + X_1 - X_1^2) - X_3(\frac{k}{k_o}[1 - X_1] - X_1 + X_1^2) = 0. \tag{45}$$

Minimizing the objective function Equation (37), subject to the four constraint equations, Equations (39), (42), (43), and (45), constitutes the funnel/gate minimum cost design

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optimization problem. The complete nonlinear formulation is summarized below and contains five primary decision variables, X_1, X_2, ℓ, L, and X_5.

$$\text{Total funnel/gate costs} = 4E_1X_2 + 2E_2\ell + 2E_3BX_1 + E_{11}B(\ell + 2L) + E_{12}QT \qquad (46)$$

subject to:

$$BX_1\ell X_5 - \frac{QT}{\theta} = 0 \qquad (47)$$

$$X_5^2(1 - X_1) - \Phi_1^2(1 - X_1) - \frac{2QL}{kB}\ln[X_1] = 0. \qquad (48)$$

$$X_2^2 - \frac{B^2}{4}(1 - 2X_1 + X_1^2) - L^2 = 0. \qquad (49)$$

$$2X_5(X_1\ln[X_1] + X_1 - X_1^2) - X_3\left(\frac{k}{k_o}[1 - X_1] - X_1 + X_1^2\right) = 0. \qquad (50)$$

LAGRANGIAN OPTIMIZATION

The above cost minimization formulation is a nonlinear optimization problem. Because this formulation contains only equality constraints (i.e., no inequalities), a solution can be obtained readily by recasting the problem as a Lagrangian optimization formulation. The first step of the approach is to formulate the Lagrangian, L_a, by combining the objective function and

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all the constraints. Thus,

$$L_a = 4E_1X_2 + 2E_2\ell + 2E_3BX_1 + E_{11}B(\ell + 2L) + E_{12}QT$$

$$+ X_6\left[BX_1\ell X_5 - \frac{QT}{\theta}\right] + X_7\left[X_5^2(1 - X_1) - \Phi_1^2(1 - X_1) - \frac{2QL}{kB}\ln[X_1]\right]$$

$$+ X_8\left[X_2^2 - \frac{B^2}{4}(1 - 2X_1 + X_1^2) - L^2\right]$$

$$+ X_9\left[2X_5(X_1\ln[X_1] + X_1 - X_1^2) - X_3(\frac{k}{k_o}[1 - X_1] - X_1 + X_1^2)\right] \qquad (51)$$

where X_6, X_7, X_8, and X_9 = Lagrangian multipliers.

The next step to reformulating the optimization problem is to derive nine equations from differentiating L_a with respect to each of the five original decision variables and each of the four Lagrangian multipliers.

$$F_1 = \frac{\partial L_a}{\partial X_1} = 2E_3B + X_6B\ell X_5 - X_7\left[X_5^2 - \Phi_1^2 + \frac{2QL}{kBX_1}\right] + \frac{X_8B^2}{4}(2 - 2X_1)$$

$$+ 2LX_9\Big(\ln[X_1] + 2. - 2X_1\Big) + \ell X_9\left[\frac{k}{k_o} + 1. - 2X_1\right] = 0 \tag{52}$$

$$F_2 = \frac{\partial L_a}{\partial X_2} = E_1 + 2X_8 X_2 = 0 \tag{53}$$

$$F_3 = \frac{\partial L_a}{\partial \ell} = 2E_2 + E_{11}B + BX_6 X_1 X_5 - X_9\left[\frac{k}{k_o}(1 - X_1) - X_1 + X_1^2\right] = 0 \tag{54}$$

$$F_4 = \frac{\partial L_a}{\partial L} = 2E_{11}B - 2LX_8 + 2X_9[X_1 \ln(X_1) + X_1 - X^2] = 0 \tag{55}$$

$$F_5 = \frac{\partial L_a}{\partial X_5} = BX_6 X_1 \ell + 2X_7 X_5(1 - X_1) = 0 \tag{56}$$

$$F_6 = \frac{\partial L_a}{\partial X_6} = BX_1 X_5 \ell - \frac{TQ}{\theta} = 0 \tag{57}$$

$$F_7 = \frac{\partial L_a}{\partial X_7} = (X_5^2 - \Phi_1^2)(1 - X_1) - \frac{2QL}{kB}\ln(X_1) = 0 \tag{58}$$

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$$F_8 = \frac{\partial L_a}{\partial X_8} = X_2^2 - \frac{B^2}{4}(1 - 2X_1 + X_1^2) - L^2 = 0 \tag{59}$$

$$F_9 = \frac{\partial L_a}{\partial X_9} = 2L\left[X_1 \ln(X_1) + X_1 - X_1^2\right] - X_3\left[\frac{k}{k_o}(1 - X_1) - X_1 + X_1^2\right] = 0 \tag{60}$$

Equations (52) - (60) constitute the Lagrangian cost optimization model comprised of nine nonlinear equations with nine unknowns (the five original decision variables and the four Lagrangian multipliers). These equations can be solved using a generalized Newton-Raphson algorithm (Smith, Henton, and Lewis, 1983). Assuming a solution is found to the above nine equations, that solution represents a stationary point that may or may not represent the minimum cost solution. To facilitate the Newton-Raphson algorithm in the search for the minimum cost solution, initial estimates of all variables are chosen which are thought to reflect values close to the minimum cost solution. Hence, the Newton-Raphson algorithm begins an iterative search for the optimum funnel/gate design (lowest cost) beginning with variable values that reflect a close approximation of optimum solution.

SUMMARY

In the first half of this Section a funnel/gate cost estimation model was developed to identify minimum cost designs subject to four constraints: one that defines the desired hydraulic retention time in the gate, one that defines the funnel wall length in terms of other system dimensions, and two that serve as hydraulic constraints. Costs considered in the model include land costs, costs per unit length of funnel walls, costs per unit length of gate, costs per unit width of gate, and costs associated with the reactive medium used in the gate.

The second half of this Section was devoted to recasting the general cost model into a Lagrangian optimization model. As a result of this reformulation, the optimization problem was reduced to that of solving a system of nine nonlinear equations [Equations (52) to (60)] with nine unknowns. Recommendations were given as to how the nine equations could be solved.

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SECTION V

FUNNEL/GATE DESIGN MODEL (FGDM)

In this chapter two objectives will be achieved. The first, is to provide a brief overview of the Funnel/Gate Design Model (FGDM) software. The second objective is to step through an example problem using FGDM.

FGDM

FGDM is a FORTRAN program developed to ascertain feasible dimensions of funnel/gate systems and also identify the lowest cost design. Feasible is defined here to include designs that are consistent with the transport and hydraulic theories outlined in Sections 2 and 3. The software includes a primary control program, FGDM.for, and four subroutines, TRANS.for, HYD.for, OPTI.for and GAUSSJ.for. During execution, subroutine TRANS.for is first called, then HYD.for, and finally OPTI.for. GAUSSJ.for is a Gauss-Jordan elimination algorithm with full pivoting that was developed by Press, Flannery, Teukolsky, and Vetterling (1990): GAUSSJ.for is called directly by OPTI.for. Each subroutine writes results to a single output file. The structure of the program is such that new subroutines may be substituted for existing versions without affecting other components of FGDM. The program requires one input file and produces one output file. In addition, it writes to the screen much of the same design information written to the output file. Section 6 provides a complete listing of the program along with examples of input and output files.

FGDM.for is the primary control program that reads the input file, dimensions several common block arrays and calls subroutines TRANS.for, HYD.for, and OPTI.for. This program also prompts the user for both input and output file names. Initially FGDM.for opens and reads the input file and then calls subroutine TRANS.for to perform contaminant fate and transport simulations in the gate. TRANS.for returns control to FGMD.for with an estimate of the critical hydraulic residence time for the gate. Next, FGMD.for calls the hydraulic design subroutine HYD.for to develop several funnel/gate designs using the aforementioned hydraulic residence time in each design. From a list of width ratios, b/B, specified in the input file, HYD.for

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formulates one system design for each width ratio. HYD.for also estimates the cost of each design and then returns control to FGMD.for. Finally, FGMD.for calls subroutine OPTI.for to search for the minimum cost system. OPTI.for initiates this search using the dimensions of the lowest cost system identified by HYD.for. Once OPTI.for finds the true minimum cost system configuration, it returns control to FGDM.for and the program terminates. Additional details regarding FGDM.for can be obtained reading the documented code (See Section 6).

TRANS.for is a contaminant fate and transport subroutine that ascertains the critical hydraulic residence time, T, in the gate using an iterative algorithm. The subroutine begins the iterative search by equating the hydraulic residence time, $T = DT$, where $DT = $ a time step specified in the input file. Next, the TRANS.for solves Equations (5), (8), (11), and (17) and then checks to determine whether calculated values for C_1, C_2, C_3, or C_4 exceed respective water quality standards STD1, STD2, STD3, or STD4. If any of the four standards are exceeded, the subroutine increases the value of T by an increment equal to DT (now $T = 2 \cdot DT$) and then reevaluates Equations (5), (8), (11), and (17) for comparison against water quality standards. This iterative process continues (and the value of T is increased after each iteration) so long as any of the calculated contaminant levels, C_1, C_2, C_3, or C_4, exceed their respective water quality standard. The iterative search stops when a value T is found that produces C_1, C_2, C_3, and C_4 values less-than-or-equal-to pertinent water quality standards. When the search has terminated, $T = $ the critical hydraulic residence time. During the search for this residence time, TRANS.for writes to an output file C_1, C_2, C_3, and C_4 values calculated for each value of T evaluated. Finally, before it returns control to FGFM.for, it writes to the output file the value of the critical hydraulic residence time.

HYD.for is the hydraulic subroutine that generates feasible funnel/gate designs. In this application, the subroutine takes the critical hydraulic residence time produced by TRANS.for to generate several systems designs. Specifically, the subroutine solves Equations (24) through (28) using the iterative design algorithm described in Section 3. Each design is created using a unique width ratio, b/B, obtained from a list specified in the input file. From the list of specified b/B values, only ratios greater than the hydraulic conductivity ratio, k/k_o, are used; it may be recalled from Christensen and Hatfield (1994) that infeasible designs are obtained for $b/B \leq k/k_o$.

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HYD.for also calculates the cost of each design using Equation (37). During execution, HYD.for writes to the output file the cost and design dimensions of each funnel/gate system configured.

OPTI.for is the subroutine used to identify the minimum cost funnel/gate design. Essentially this subroutine employs a generalized Newton-Raphson algorithm (Smith, Hinton, and Lewis, 1983) combined with a Gauss-Jordan elimination algorithm with full pivoting (Press, Flannery, Teukolsky, and Vetterling, 1990) to solve the system of nine nonlinear equations [Equations (52) - (60)] of the Lagrangian cost model. OPTI.for initiates an iterative search for the minimum cost design using the dimensions of the lowest cost system identified by HYD.for. During the search process, OPTI.for calls subroutine GAUSSJ.for to solve a new system of equations generated from the application of the Newton-Raphson algorithm to the original aforementioned nine nonlinear equations. Once OPTI.for finds the true minimum cost system configuration, the cost and dimensions of this system are written to the screen and to the output file. Finally, the subroutine writes to the output file the surface areas associated with the funnel walls, the longitudinal gate walls, and the transverse gate walls. These surface areas can be used to verify that appropriate values have been used to define cost parameters, C_{sfgl}, C_{sffw}, and C_{sfgw} in the input file.

EXAMPLE PROBLEM

To demonstrate FGDM, a problem example was formulated. Consider a site with a plume that is 49 meters wide. The plume contains PCE and TCE with a maximum concentration of each at 5000 μg/l. The local phreatic surface is 0.5 meters below ground surface, and the depth to the aquiclude is 5.5 meters; thus, $\phi_1 = 5$ m . The local groundwater flow gradient is $d\phi/dx = -0.005$ in an aquifer with an estimated hydraulic conductivity of k = 4.32 m/d.

The suggested groundwater remediation approach for the site is to intercept and treat the polluted groundwater using a funnel/gate. The applicable system performance standard is for water exiting the gate to meet water quality standards of 5 μg/l PCE, 5 μg/l TCE, 70 μg/l DCE, and 1 μg/l vinyl chloride.

To initiate an investigation of feasible system designs, typical funnel/gate parameters are assumed (i.e., degradation parameters, gate porosities, gate widths, and gate hydraulic

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conductivities). The gate porosity and hydraulic conductivity are assumed to be, respectively, θ = 0.45 and k_o = 43.2 m/d. The gate width, b, is determined by the value of the funnel width B and the gate to funnel width ratio, b/B. FGDM can be used to study a suite of up to 10 funnel/gate designs. Each design reflects a unique b/B ratio; however, FGDM ignores ratios with values less than the hydraulic conductivity ratio, k/k_o. As for the funnel width, B, this parameter is estimated in advance assuming a reasonable capture efficiency, i.e., 80 percent (see example validation problems presented in Section 3). Under this assumption, a funnel entrance width B = 61 meters is needed to intercept a plume 49 meters wide. Finally, there are degradation parameters, Gillham (1995) suggests the following first-order estimates: λ_{1a} = 36.9 d^{-1} and λ_{1b} = 0.0 d^{-1} for PCE; λ_{2a} = 3.69 d^{-1} and λ_{2b} = 33.18 d^{-1} for TCE; λ_{3a} = .83 d^{-1} and λ_{1b} = 0.0 d^{-1} for PCE; and λ_{1a} = .83 d^{-1} for vinyl chloride.

In this example, it is assumed that both funnel and gate structures will be constructed from sheet piles. Since the aquiclude exists 5.5 meters below ground surface, these piles will be driven to a total depth, d = 6 meters (allowing 0.5 meters of sheet pile depth as a key into the aquitard). The values of applicable sheet pile cost parameters can be obtained from Section 4. The reactive gate material costs are taken to equal \$1,725 m $^{-3}$, while land costs are assumed small.

The above information was incorporated into an FGDM input file shown on the next page. Line numbers were added to the right of the file text for quick referencing. Line 3 contains water quality standards STD1 (5 μg/l), STD2 (5 μg/l), STD3 (70 μg/l), and STD4 (1 μg/l) for respective contaminants C_1 (PCE), C_2 (TCE), C_3 (DCE), and C_4 (vinyl chloride). The last number appearing in line 3 is the time step, DT (0.1 days), used in the subroutine TRANS.for, to increase the hydraulic residence time between iterative calculations of C_1, C_2, C_3, and C_4. The assumed funnel width, B (61 m), the hydraulic gradient, $d\phi/dx$ (-0.005), the saturated aquifer thickness, ϕ_1 (5 m), and the aquifer hydraulic conductivity, k (4.32 m/d) are written in line 7. The gate porosity, θ (0.45), the aquifer gate hydraulic conductivity ratio k/k_o (0.1), and the depth of the funnel/gate walls d (6 meters) are listed on line 11. Lines 17 and 21

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Example Input File:

Data	Line Number

STD1 [ug/l] STD2 [ug/l] STD3 [ug/l] STD4 [ug/l] DT(TIMESTEP) [DAYS] — 1
* — 2
  5.0   5.0   70.0   1.0   .1 — 3
* — 4
FUNNEL WIDTH [M] GRADIENT AQU. THICKNESS [M] AQU. HYDRAULIC COND. [M/d] — 5
* — 6
    61.   - 0.005   5.   4.32 — 7
* — 8
GATE POROSITY HYDRAULIC COND. RATIO (AQUIFER/GATE) DEPTH OF SYSTEM WALLS [M] — 9
* — 10
    .45   .1   6. — 11
* — 12
VARIOUS RATIOS OF GATE WIDTH TO PLUME WIDTH b/B EXAMINED — 13
* — 14
BR(1) BR(2) BR(3) BR(4) BR(5) — 15
* — 16
.02   .05   .1   .2   .4 — 17
* — 18
BR(6) BR(7) BR(8) BR(9) BR(10) — 19
* — 20
.5   .6   .7   .8   .9 — 21
* — 22
****DATA PLUME CONTAMINANT CONCENTRATIONS AND DEGRADATION PARAMETERS — 23
* — 24
PLUME C1 CONC. [ug/l] LAMBDA 1A [1/DAY] LAMBDA 1B [1/DAY] — 25
* — 26
    5000.   36.9   0. — 27
* — 28
PLUME C2 CONC. [ug/l] LAMBDA 2A [1/DAY] LAMBDA 2B [1/DAY] — 29
* — 30
    5000.   3.69   33.18 — 31
* — 32
PLUME C3 CONC. [ug/l] LAMBDA 3A [1/DAY] LAMBDA 3B [1/DAY] — 33
* — 34
    0.   .8318   0. — 35
* — 36
PLUME C4 CONC. [ug/l] LAMBDA 4A [1/DAY] — 37
* — 38
    0.   .8318 — 39
* — 40
* READ IN COSTS COEFFICIENTS: [IN UNITS OF THOUSANDS OF DOLLARS] — 41
*   CSFFW = COST PER UNIT AREA OF FUNNEL WALL MATERIAL — 42
*   CSFGL = COST PER UNIT AREA OF LONGITUDINAL GATE WALL — 43
*   CSFGW = COST PER UNIT AREA OF TRANSVERSE GATE WALL — 44
*   E11 = LAND COSTS PER UNIT AREA — 45
*   E12 = REACTIVE MEDIA COSTS PER UNIT VOLUME — 46
* — 47
 CSFFW   CSFGL   CSFGW   E11   E12 — 48
* — 49
 .193   .193   .193   .001   1.725 — 50
* — 51
* READ IN INITIAL ESTIMATES OF LAGRANGIAN MULTIPLIERS, X6, X7, X8, AND X9 — 52
* — 53
X6 X7 X8 X9 — 54
* — 55
1.   1.   1.   10. — 56

comprise a listing of width ratios, b/B, to be evaluated with FGDM. The maximum PCE concentration C_{10} = 5000 µg/l and pertinent decay parameters λ_{1a} = 36.9 d^{-1} and λ_{1b} = 0.0 d^{-1} for PCE are written on line 27. On line 31 there is the maximum TCE concentration C_{20} = 5000 µg/l and associated decay parameters λ_{2a} = 3.69 d^{-1} and λ_{2b} = 33.18 d^{-1}. Line 35 lists the maximum plume concentration for DCE C_{30} = 0 µg/l and decay parameters λ_{3a} = .83 d^{-1} and λ_{3b} = 0. d^{-1}. For vinyl chloride, input file line 39 contains the maximum plume concentration C_{40} = 0 µg/l and decay parameter λ_{4a} = .83 d^{-1}. The next important data line is number 50. This line contains values for cost parameters C_{sffw} = .193, C_{sfgl} = .193, and C_{sfgw} = .193. In addition, this line includes the cost per unit area of land, E_{11} = .001, and the cost per unit volume of reactive gate material, E_{12} = 1.725 thousand dollars/m^3. Note, all cost coefficients are expressed in terms of thousands of dollars (compare with Table 1). Finally, there is line 56 which contains initial estimates of the values of Lagrangian multiplier X_6 =1., X_7 = 1., X_8 = 1., and X_9 = 10. Unless there are severe convergence problems, line 56 need not be changed between applications. If these problems do occur, it is suggested that the user look at the output file first. Output will exist from HYD.for, which may reveal that a low cost system doesn't exist. Making a plot of system costs versus system width ratios, b/B, (see Figure 10 next section) may reveal a flat or monotonic curve that has no minimum value; this would explain why OPTI.for failed to converge on a low cost system.

Using the above input file, FGDM generates an output file that may be divided into the three respective sections produced from subroutines TRANS.for, HYD.for and OPTI.for. Shown on the next page is an abbreviated output file from the above example problem. The first section is generated from subroutine TRANS.for. This section contains five printed columns, the first being the hydraulic residence time T, and the remaining four reflecting calculated values of contaminants C_1, C_2, C_3, and C_4 (in this case PCE, TCE, DCE, and vinyl chloride). The end of the first section is marked by a statement:

CRITICAL HYDRAULIC RESIDENCE TIME =   11.10 [DAY]

This statement indicates the value of the critical hydraulic residence time in the gate determined by the conditions defined in the example problem. Section one results showed PCE, TCE, and DCE concentrations decreased to performance standards in the gate long before vinyl chloride;

however, by day 11.1 vinyl chloride decreased below the 1.0 µg/l standard. Figure 8 is a plot of the data from the first section showing PCE, TCE, DCE, and vinyl chloride concentrations as a function of gate hydraulic residence time. Figure 8 clearly shows the degradation of PCE and TCE and the subsequent production/degradation of DCE and vinyl chloride. Figure 9 contains only the first two days of data used in Figure 8. This figure illustrates more clearly the rapid disappearance of PCE and TCE.

The second section of the output file is generated by subroutine HYD.for. Each line of this section contains the dimensions and the cost of a single feasible funnel/gate system for a b/B ratio specified in the input file. It should be noted that b/B ratios 0.02, 0.05, and 0.1 were listed in the input file, but output lines were not generated by HYD.for because they are less than $k/k_o = 0.1$. The first three columns of output in this section are gate widths, b, lengths, ℓ, and gate volumes. The basic length unit is meters. It may be observed that the gate volume is constant between designs, while gate length and width vary. A constant gate volume is expected because the hydraulic residence time is a constant. The next two columns give funnel wall lengths, X_2 and projected funnel wall lengths, L. Under the next heading of 'Dimensionless Parameters' there is a column for gate/funnel width ratios, b/B and another for length ratios, L/ℓ; these parameters found relevance in Christensen and Hatfield (1994). Finally, the last column contains total system costs expressed as thousands of dollars. Figure 10 is a plot of the total system cost versus the width ratio, b/B. Clearly, Figure 10 identifies the lower cost systems as those with gate/funnel width ratios ranging from 0.5 to 0.7. Given that funnel/gate capture efficiency increases with the value of the width ratio, b/B (recall validation studies in Section 3), it may be desirable to select among the lower cost designs, the one with the largest width ratio.

The beginning of the third and last section of the output file is marked by the heading:

********* MINIMUM COST DESIGN ********

This section is written by subroutine OPTI.for and has initially the same format as the second output section. The third section initially lists the dimensions and cost of the true minimum cost design. The total cost of this design is $424,000, and it has the following dimensions:

40

Example Output File:

TIME	C1	C2	C3	C4
[DAY]	[ug/l]	[ug/l]	[ug/l]	[ug/l]
.00	5000.	5000.	.00	.00
.10	124.8	586.6	879.91	48.15
.20	3.12	26.22	873.98	115.50
.30	.08	.94	806.89	173.34
.40	.00	.03	742.58	221.27
.50	.00	.00	683.31	260.45
.60	.00	.00	628.77	291.96
.70	.00	.00	578.59	316.79
.80	.00	.00	532.41	335.79
.	.	.	.	.
.	.	.	.	.
.	.	.	.	.
10.70	.00	.00	.14	1.25
10.80	.00	.00	.13	1.16
10.90	.00	.00	.12	1.08
11.00	.00	.00	.11	1.00
11.10	.00	.00	.10	.93

CRITICAL HYDRAULIC RESIDENCE TIME = 11.10 [DAY]

GATE			FUNNEL		DIMENSIONLESS PARAMETERS		TOTAL COSTS
WIDTH	LENGTH	VOLUME	LENGTH	PROJECTED LENGTH	b/B	L/l	THOUSANDS OF DOLLARS
[M]	[M]	[M^3]	[M]	[M]			
12.20	2.67	162.50	24.41	.66	.20	.25	428.
24.40	1.33	162.50	18.32	.95	.40	.71	425.
30.50	1.07	162.50	15.29	1.11	.50	1.04	424.
36.60	.89	162.50	12.27	1.34	.60	1.50	424.
42.70	.76	162.50	9.31	1.73	.70	2.27	424.
48.80	.67	162.50	6.60	2.53	.80	3.78	426.
54.90	.60	162.50	5.80	4.93	.90	8.29	436.

********** MINIMUM COST DESIGN ********

GATE			FUNNEL		DIMENSIONLESS PARAMETERS		TOTAL COSTS
WIDTH	LENGTH	VOLUME	LENGTH	PROJECTED LENGTH	b/B	L/l	THOUSANDS OF DOLLARS
[M]	[M]	[M^3]	[M]	[M]			
36.60	.89	162.78	12.27	1.34	.60	1.50	424.

TOTAL FUNNEL WALL AREA [M^2] = 294.6
TOTAL GATE WIDTH WALL AREA [M^2] = 439.2
TOTAL GATE LENGTH WALL AREA [M^2] = 10.7
TOTAL FUNNEL/GATE WALL AREA [M^2] = 744.4
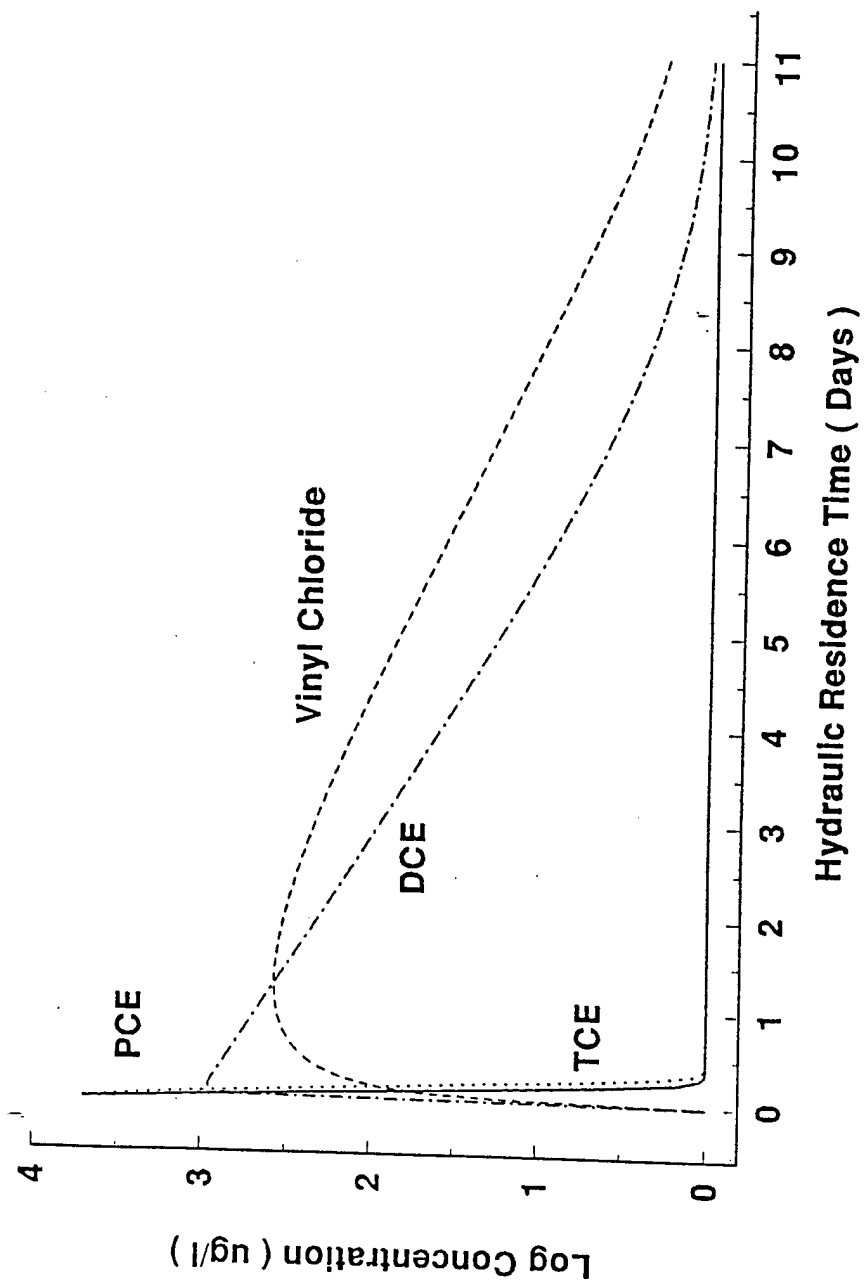
Figure 8. Funnel/Gate Design Example, Selected Contaminant Fate in the Gate.
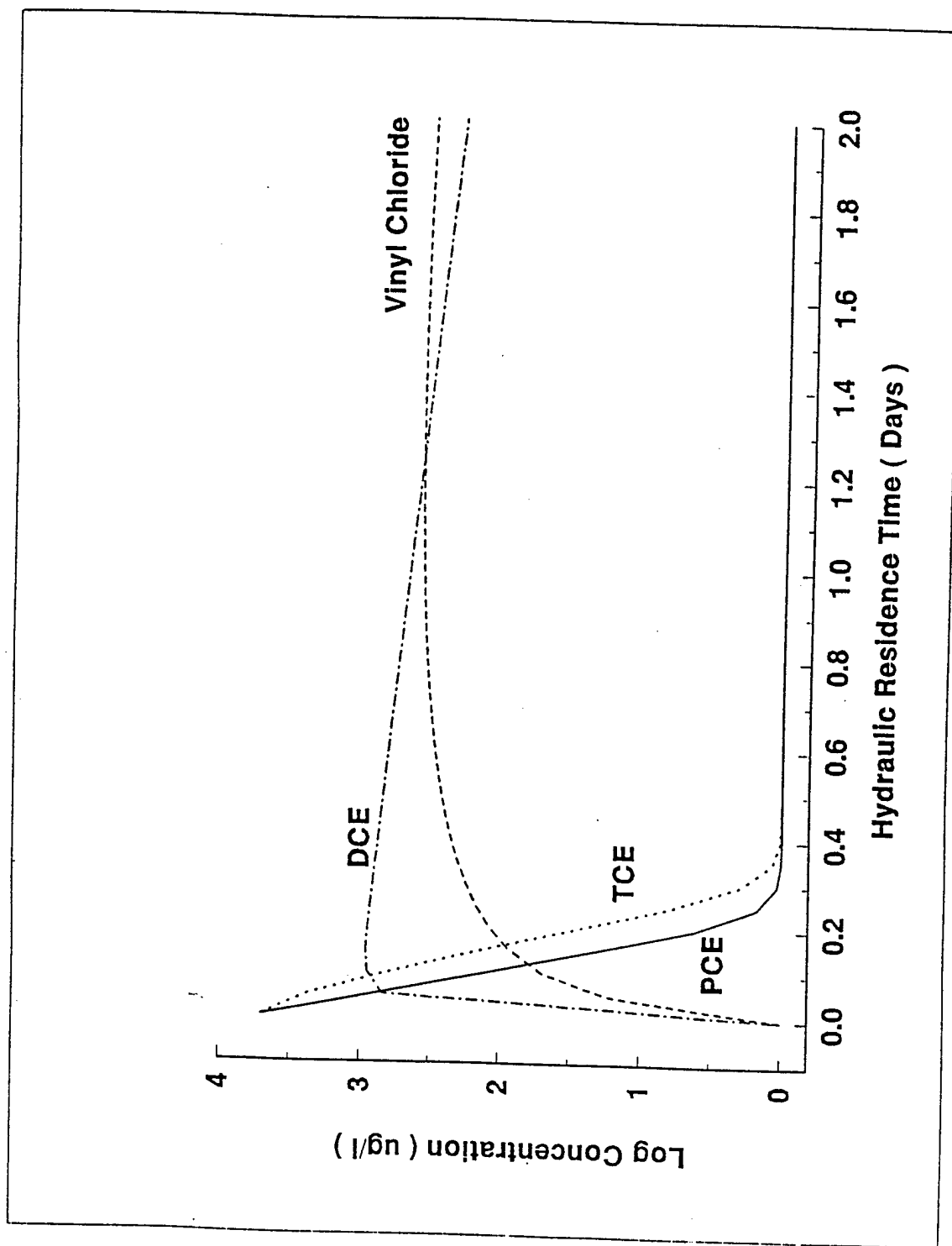
Figure 9. Funnel/Gate Design Example, Selected Contaminant Fate in the Gate.
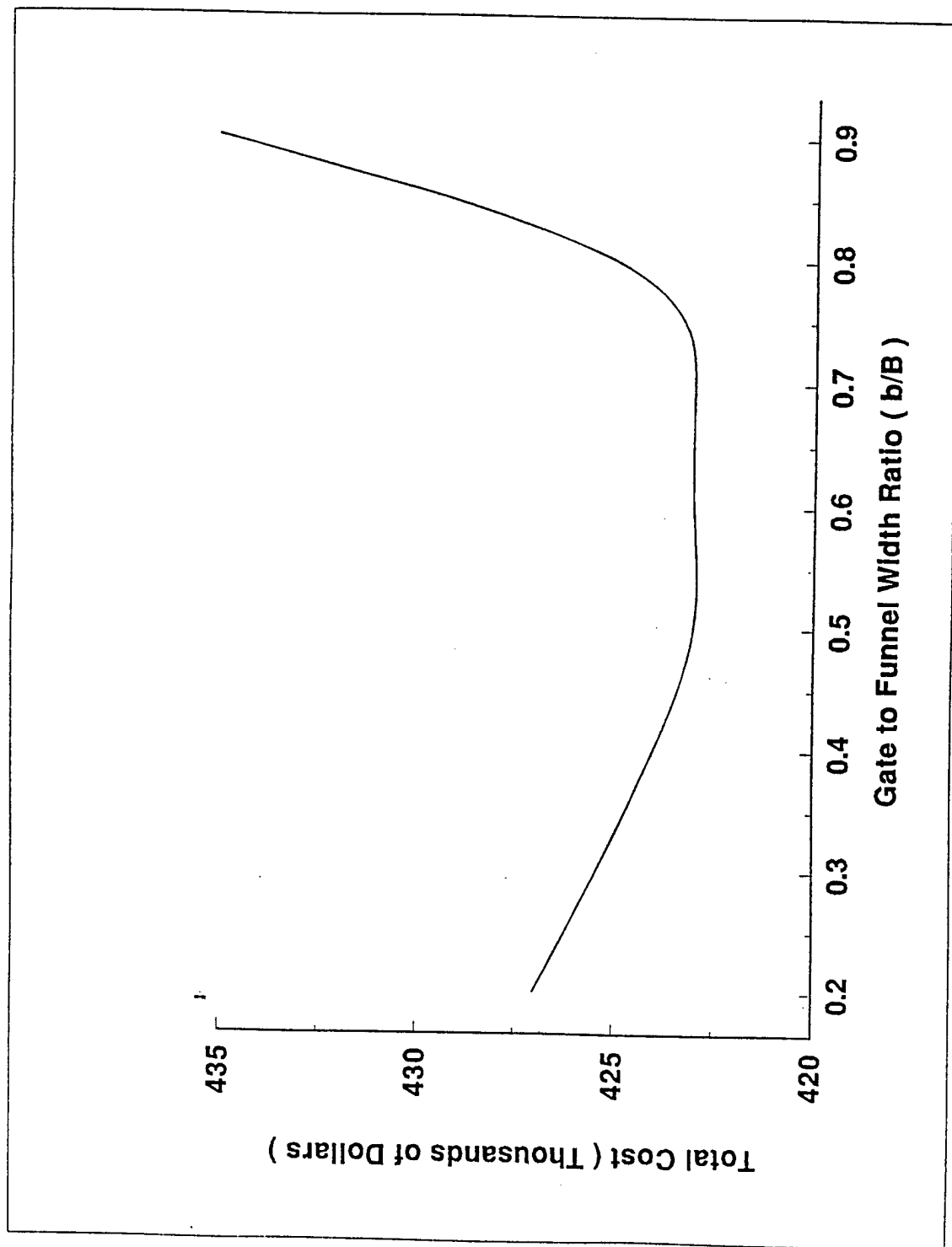
Figure 10. Funnel/Gate Design Example, Total System Cost.

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$B = 61.\ m$

$b = 36.6\ m$

$\ell = .89\ m$

$L = 1.39\ m$

The last four lines of output give total calculated areas for the funnel walls, the transverse gate walls, the longitudinal gate walls, and the summation of all walls. These areas can be combined as needed to be certain estimated system areas are consistent with the unit costs used from Table 1. A quick view of Table 1 verifies that the projected area of 744.4 m^2 is well within the specified range of 465 - 860 m^2 used to select values for unit cost coefficients, C_{sffw}, C_{sfgl}, and C_{sfgw}.

FGDM CODE LISTING

Subroutine FGDM.for:

```
****************************************************************************
*
*   FROM: KIRK HATFIELD
*       DEPARTMENT OF CIVIL ENGINEERING
*       UNIVERSITY OF FLORIDA
*       GAINESVILLE, FLORIDA 32611  U.S.A.
*
****************************************************************************
****************************************************************************
     PROGRAM FGDM
****************************************************************************
****************************************************************************
*
*   Variable Declarations
*
****************************************************************************
C
     IMPLICIT DOUBLE PRECISION (A-H, O-Z)
     DIMENSION BR(10),GATEL(10),VOL(10),WING(10),RL(10),
    /TCOST(10),ANGLE(10),A(9,9),B(9,2),XX(4)
     COMMON A,B,BR,GATEL,VOL,WING,RL,TCOST,ANGLE,XX
C  READ IN THE NAMES OF THE INPUT AND OUTPUT FILES
C
     CHARACTER*70 INFIL,OUTFIL,INPUT,OUTPUT
     CHARACTER*1 HEADER
     WRITE(6,*) 'NAME OF INPUT FILE'
     READ (5,5) INFIL
     INPUT=INFIL
     WRITE(6,*) 'NAME OF OUTPUT FILE'
5    FORMAT(A70)
     READ (5,5) OUTFIL
     OUTPUT = OUTFIL
     OPEN (UNIT=11,FILE=INPUT,STATUS='OLD')
     OPEN (UNIT=12,FILE=OUTPUT,STATUS='UNKNOWN')
```

```
C READING IN HEADER (IGNORE)
      READ (11,70)HEADER
 70   FORMAT(A1)
      READ (11,70)HEADER
C READ IN WATER QUALITY STANDARDS IN (ug/l), FOR PCE = STD1, TCE = STD2,
C DCE = STD3, AND VINYL CHLORIDE = STD4
C READ IN TIME STEP INCREMENT = DT, IN DAYS
C
      READ (11,*)STD1,STD2,STD3,STD4,DT
      READ (11,70)HEADER
C
C THE PERMEABILITY OF THE AQUIFER = RKP, IN METERS/DAY
C SATURATED THICKNESS = RPHI1, IN METERS
C THE AQUIFER GRADIENT = GRAD, IN METERS
C THE PLUME WIDTH = BIGB, IN METERS
C
      READ (11,70)HEADER
      READ (11,70)HEADER
      READ (11,*)BIGB,GRAD,RPHI1,RKP
      READ (11,70)HEADER
      Q = -GRAD*BIGB*RKP*RPHI1
C
C THE POROSITY OF THE GATE = THETA
C THE RATIO OF AQUIFER TO GATE PERMEABILITY = RATIOK
C THE DEPTH TO AQUICLUDE OR DEPTH OF FUNNEL/GATE WALLS
C
      READ (11,70)HEADER
      READ (11,70)HEADER
      READ (11,*)THETA,RATIOK,DEPTH
      READ (11,70)HEADER
C
C THE GATE WIDTH TO PLUME WIDTH RATIOS, b/B EXAMINED = BR(I)
C
      READ (11,70)HEADER
      READ (11,70)HEADER
      READ (11,70)HEADER
      READ (11,70)HEADER
      READ (11,*)BR(1),BR(2),BR(3),BR(4),BR(5)
      READ (11,70)HEADER
      READ (11,70)HEADER
      READ (11,70)HEADER
      READ (11,*)BR(6),BR(7),BR(8),BR(9),BR(10)
      READ (11,70)HEADER
```

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```
C
C THE INITIAL CONCENTRATION OF PCE = C10 IN ug/l, AND PCE DEGRADATION
C RATE
C COEFFICIENTS LAMBDA 1a = RLM1A AND LAMBDA 1b = RLM1B, IN [ 1/DAYS ]
C
      READ (11,70)HEADER
      READ (11,70)HEADER
      READ (11,70)HEADER
      READ (11,70)HEADER
      READ (11,*)C1O,RLM1A,RLM1B
      READ (11,70)HEADER
C
C THE INITIAL CONCENTRATION OF TCE = C20 IN ug/l, AND TCE DEGRADATION
C RATE
C COEFFICIENTS LAMBDA 2a = RLM2A AND LAMBDA 2b = RLM2B, IN [ 1/DAYS ]
C
      READ (11,70)HEADER
      READ (11,70)HEADER
      READ (11,*)C2O,RLM2A,RLM2B
      READ (11,70)HEADER
C
C THE INITIAL CONCENTRATION OF DCE = C30 IN ug/l, AND DCE DEGRADATION
C RATE
C COEFFICIENTS LAMBDA 3a = RLM3A AND LAMBDA 3b = RLM3B, IN [ 1/DAYS ]
C
      READ (11,70)HEADER
      READ (11,70)HEADER
      READ (11,*)C3O,RLM3A,RLM3B
      READ (11,70)HEADER
C
C THE INITIAL CONCENTRATION OF VINYL CHLORIDE = C40 IN ug/l, AND
C THE VINYL CHLORIDE DEGRADATION RATE COEFFICIENT LAMBDA 4a = RLM3A,
C IN [ 1/DAYS ]
C
      READ (11,70)HEADER
      READ (11,70)HEADER
      READ (11,*)C4O,RLM4A
      READ (11,70)HEADER
C
C READ IN COSTS COEFFICIENTS:
C      CSFFW = COST PER UNIT AREA OF FUNNEL WALL MATERIAL
C      CSFGL = COST PER UNIT AREA OF LONGITUDINAL GATE WALL
C      CSFGW = COST PER UNIT AREA OF TRANSVERSE GATE WALL
```

48

```
C      E11 = LAND COSTS PER UNIT AREA
C      E12 = REACTIVE MEDIA COSTS PER UNIT VOLUME
C
       READ (11,70)HEADER
       READ (11,70)HEADER
       READ (11,70)HEADER
       READ (11,70)HEADER
       READ (11,70)HEADER
       READ (11,70)HEADER
       READ (11,70)HEADER
       READ (11,70)HEADER
       READ (11,70)HEADER
       READ (11,*) CSFFW,CSFGL,CSFGW,E11,E12
C      E1 = COST PER UNIT LENGTH OF FUNNEL WING WALL
C      E2 = COST PER UNIT LENGTH OF GATE LENGTH
C      E3 = COST PER UNIT GATE WIDTH
       E1 = CSFFW*DEPTH
       E2 = CSFGL*DEPTH
       E3 = CSFGW*DEPTH
       READ (11,70)HEADER
C
C READ IN INITIAL ESTIMATES OF LAGRANGIAN MULTIPLIERS (USE SUGGESTED
C VALUES FROM REPORT)
C
       READ (11,70)HEADER
       READ (11,70)HEADER
       READ (11,70)HEADER
       READ (11,70)HEADER
       READ (11,*) XX6,XX7,XX8,XX9
C
C ***************
C
C FIRST WE SOLVE THE TRANSPORT PROBLEM, IN WHICH WE DETERMINE THE
C MINIMUM HYDRAULIC RESIDENCE
C TIME NEEDED TO MEET WATER QUALITY STANDARDS AT THE GATE EXIT
C    THE SUBROUTINE RETURNS WITH A VALUE FOR THE MINIMUM DETENTION
C    TIME, TD,
C    NEEDED TO ACHIEVE SUFFICIENT DEGRADATION SUCH THAT WATER
C    QUALITY STANDARDS
C    ARE MET
C
       CALL TRANS(STD1,STD2,STD3,STD4,DT,C1O,RLM1A,RLM1B,C2O,RLM2A,
      /RLM2B,C3O,RLM3A,RLM3B,C4O,RLM4A,TD)
```

49

```
C
C ***************
C ***************
C
C NOW WE SOLVE FOR VARIOUS FUNNEL/GATE DESIGN CONFIGURATIONS THAT
C PRODUCE SUFFICIENT
C HYDRAULIC RESIDENCE TIME, TD, WITHIN THE REACTIVE GATE. IN ADDITION,
C  A FIRST ESTIMATE
C IS FOUND FOR THE LEAST COST DESIGN IS FOUND.
C
    CALL HYD(TD,BR,GATEL,VOL,WING,RL,RATIOK,RKP,RPHI1,Q,BIGB,TCOST
    /,THETA,E1,E2,E3,E11,E12,K)
C
C ****************
C
C NOW WE DETERMINE THE FUNNEL/GATE DESIGN CONFIGURATION OF
C MINIMUM COST
C
    CALL OPTI(BIGB,TD,Q,THETA,RPHI1,RKP,RATIOK,BR(K),WING(K),GATEL(K),
    /RL(K),E1,E2,E3,E11,E12,XX6,XX7,XX8,XX9,DEPTH)
C
C ***************
 91   PRINT*,'THE END'
    CLOSE(UNIT=11)
    CLOSE(UNIT=12)
    STOP
    END
```

50

Subroutine TRANS.for:

```
C
C  SUBROUTINE TRANS SIMULATES TRANSPORT THROUGH THE GATE OF A
C  FUNNEL/GATE SYSTEM
C
C PARAMETERS USED BY THE SUBROUTINE INCLUDE:
C    WATER QUALITY STANDARDS IN (ug/l), FOR PCE = STD1, TCE = STD2,
C    DCE = STD3, AND VINYL CHLORIDE = STD4,
C    TIME STEP INCREMENT = DX, IN DAYS
C    THE INITIAL CONCENTRATION OF PCE = C10, IN ug/l, AND PCE DEGRADATION
C    RATE
C    COEFFICIENTS LAMBDA 1a = RLM1A AND LAMBDA 1b = RLM1B, IN [1/DAY]
C    THE INITIAL CONCENTRATION OF TCE = C20, IN ug/l AND TCE DEGRADATION
C    RATE
C    COEFFICIENTS LAMBDA 2a = RLM2A AND LAMBDA 2b = RLM2B, IN [1/DAY]
C    THE INITIAL CONCENTRATION OF DCE = C30, IN ug/l AND DCE DEGRADATION
C    RATE
C    COEFFICIENTS LAMBDA 3a = RLM3A AND LAMBDA 3b = RLM3B, IN [1/DAY]
C    THE INITIAL CONCENTRATION OF VINYL CHLORIDE = C40, IN ug/l,
C    AND THE VINYL CHLORIDE DEGRADATION RATE COEFFICIENT LAMBDA 4a =
C    RLM4A, IN [1/DAY]
C
C    THE SUBROUTINE RETURNS WITH A VALUE FOR THE CRITICAL HYDRAULIC
C RESIDENCE TIME = X, IN DAYS
C    NEEDED TO ACHIEVE SUFFICIENT DEGRADATION SUCH THAT WATER
C QUALITY STANDARDS
C    ARE MET
     SUBROUTINE TRANS(STD1,STD2,STD3,STD4,DX,C1O,RLM1A,RLM1B,
     /C2O,RLM2A,RLM2B,C3O,RLM3A,RLM3B,C4O,RLM4A,X)
     IMPLICIT DOUBLE PRECISION (A-H, O-Z)
     CHARACTER*5 ATM
     CHARACTER*8 ATM6
     CHARACTER*13 ATM1,ATM2,ATM3,ATM4,ATM5
     CHARACTER*38 ATM7
     ATM ='TIME'
     ATM1='    C1    '
     ATM2='    C2    '
     ATM3='    C3    '
     ATM4='    C4    '
     ATM5='  [ug/l]  '
     ATM6='[ DAY ]'
C PARAMETER RJ,RK,RG,RM,RF,RH, AND RP ARE SIMPLY INTERMEDIATE
```

```
C PARAMETERS DEFINED
C IN THE THEORY SECTION OF THE REPORT AS j,k,g,m,f,h,p.
      RJ = (RLM1B+RLM1A)
      RK = RLM1A
      RG = (RLM2A+RLM2B)
      RM = (RLM3A+RLM3B)
      RF = RLM2A
      RH = RLM4A
      RP = RLM3A
C CHECK TO MAKE SURE PARMETERS ARE NEVER EQUAL
C OTHERWISE A MORE EXPLICIT SOUTION MUST BE MADE FOR ALL
C POSSIBLE COMBINATIONS OF EQUAL PARAMETER PAIRS INCLUDING RJ,RG,RM,
C AND RH.
      RJ = RJ+.000001
      RG = RG+.000002
      RH = RH+.000003
      RM = RM+.000004
C SPECIFYING THE INITIAL CONDITIONS AT THE ENTRANCE OF THE GATE OR
C WHERE THE TOTAL HYDRAULIC
C RESIDENCE TIME, X, IS ZERO, WHILE C1, C2, C3, AND C4 RESPECTIVELY
CORRESPOND TO DISSOLVED
C CONCENTRATION (IN ug/l) VARIABLES FOR PCE,TCE,DCE, AND VINYL
CHLORIDE
      X=0.0
      C1=C1O
      C2=C2O
      C3=C3O
      C4=C4O
C WRITE OUT THE HEADING FOR THE OUTPUT GENERATED BY TRANS
C
      WRITE(12,21) ATM,ATM1,ATM2,ATM3,ATM4
      WRITE(12,*) ' '
      WRITE(12,20)ATM6,ATM5,ATM5,ATM5,ATM5
      WRITE(12,*)' '
      WRITE(12,*)' '
  20  FORMAT(1X,A8,2X,4(13A))
  21  FORMAT(A8,2X,4(13A))
C WRITING OUT THE INITIAL CONDITIONS AT THE EXIT OF THE GATE
C WHICH INCLUDE THE CUMULATIVE HYDRAULIC RESIDENCE TIME, X, AND THE
C FOUR CONSTITUENT
C CONCENTRATIONS, PCE, TCE, DCE, AND VINYL CHLORIDE
      WRITE(12,68) X,C1,C2,C3,C4
C
```

```
C THIS IS THE BEGINNING OF A LOOP THAT SOLVES FOR THE CONCENTRATION
C OF EACH DISSOLVED CONSTITUENT AS THE TOTAL HYDRAULIC RESIDENCE
C TIME, X IS INCREASED BY
C AN INCREMENT, DX,....THE PROGRAM CONTINUES TO SOLVE FOR
CONSTITUENT
C CONCENTRATIONS
C FOR EVER INCREASING HYDRAULIC RESIDENCE TIMES, X, UNTIL CALCULATED
C CONSTITUENT CONCENTRATIONS
C ARE LESS-THAN-OR-EQUAL-TO PERTINENT WATER QUALITY STANDARDS
  10  X = X+DX
C THE SOLUTION TO THE FIRST REACTANT PCE (SEE REPORT)
      C1 = C1O*EXP(-RJ*X)
C THE SOLUTION TO THE  SECOND REACTANT TCE (SEE REPORT)
      TERM1 = RK*C1O
      TERM2 = (EXP(-RJ*X)-EXP(-RG*X))/(RG-RJ)
      C2 = C2O*EXP(-RG*X)+TERM1*TERM2
C THE  SOLUTION TO THE THIRD REACTANT DCE (SEE REPORT)
      RA1 = C3O-RF*C2O/(RM-RG)
      RA2 = -RF*RK*C1O/((RG-RJ)*(RM-RJ))
      RA3 = RF*RK*C1O/((RG-RJ)*(RM-RG))
      RA = RA1+RA2+RA3
      RD1 = RF*C2O/(RM-RG)
      RD2 = -RF*RK*C1O/((RG-RJ)*(RM-RG))
      RD = RD1+RD2
      RE = RF*RK*C1O/((RG-RJ)*(RM-RJ))
      C3=RA*EXP(-RM*X)+RE*EXP(-RJ*X)+RD*EXP(-RG*X)
C THE  SOLUTION TO THE FOURTH REACTANT VINYL CHLORIDE (SEE REPORT)
      TERM1 = C4O*EXP(-RH*X)
      TERM2 = RA*(EXP(-RM*X)-EXP(-RH*X))/(RH-RM)
      TERM3 = RE*(EXP(-RJ*X)-EXP(-RH*X))/(RH-RJ)
      TERM4 = RD*(EXP(-RG*X)-EXP(-RH*X))/(RH-RG)
      C4 = TERM1+RP*(TERM2+TERM3+TERM4)
C WRITING OUT THE CUMULATIVE HYDRAULIC RESIDENCE TIME, X, AND THE
C FOUR CONSTITUENT
C CONCENTRATIONS, PCE, TCE, DCE, AND VINYL CHLORIDE
      WRITE(12,68) X,C1,C2,C3,C4
  68  FORMAT(F6.2,4(3X,F10.2))
C THIS IS WHERE THE PROGRAM HAS DETERMINES IF CALCULATED
C CONSTITUENT CONCENTRATIONS
C ARE LESS-THAN-OR-EQUAL-TO PERTINENT WATER QUALITY STANDARDS
      IF(C1.GT.STD1) GO TO 10
      IF(C2.GT.STD2) GO TO 10
      IF(C3.GT.STD3) GO TO 10
```

```
      IF(C4.GT.STD4) GO TO 10
C
C THIS IS THE END OF THE LOOP THAT SOLVES FOR THE CONCENTRATIONS
C OF EACH DISSOLVED CONSTITUENT AS THE TOTAL HYDRAULIC RESIDENCE
C TIME, X IS INCREASED BY
C AN INCREMENT, DX,
C
      WRITE(12,*)' '
      ATM7 =' CRITICAL HYDRAULIC RESIDENCE TIME = '
      WRITE(12,70) ATM7,X,ATM6
 70   FORMAT(A38,2X,F6.2,2X,A8)
      WRITE(12,*)' '
C
C THE PROGRAM HAS DETERMINED THAT CALCULATED CONSTITUENT C C
CONCENTRATIONS
C ARE LESS-THAN-OR-EQUAL-TO PERTINENT WATER QUALITY STANDARDS AND
C WILL NOW RETURN WITH
C A VALUE FOR THE CRITICAL HYDRAULIC RESIDENCE TIME, X, NEEDED TO
C MEET WATER QUALITY STANDARDS

      RETURN
      END
```

Subroutine HYD.for:

```
C
C SUBROUTINE HYD CONTAINS APPROPRIATE RELATIONSHIPS TO SOLVE FOR
C VARIOUS FUNNEL/GATE DESIGN CONFIGURATIONS THAT PRODUCE
SUFFICIENT
C HYDRAULIC RESIDENCE TIME, T, WITHIN THE REACTIVE GATE.
C IN ADDITION, THIS SUBROUTINE GENERATES AN INITIAL ESTIMATE
C OF THE DESIGN THAT REPRESENT THE MINIMUM COST CONFIGURATION.
C THE PERTINENT SYSTEM DIMENSION OF THE MINIMUM COST CONFIGURATION
C ARE STORE IN SEVERAL COMMON BLOCK ARRAYS.
C
C PARAMETERS USED BY THE SUBROUTINE INCLUDE:
C    THE CRITICAL HYDRAULIC RESDENCE TIME, X, IN DAYS, PROVIDED BY
C        SUBROUTINE TRANS
C    AN ARRAY CONTAINING SEVERAL GATE WIDTH TO FUNNEL WIDTH RATIOS,
C b/B, = BR(I)
C    THE PERMEABILITY OF THE AQUIFER=RKP, IN METERS/DAY
C    SATURATED THICKNESS=RPHI1, IN METERS
C    THE AQUIFER DISCHARGE=Q (IN CUBIC METERS/DAY), ACROSS THE FUNNEL
C WIDTH
C    THE FUNNEL WIDTH=BIGB,IN METERS
C    THE POROSITY OF THE GATE = THETA
C    THE RATIO OF AQUIFER TO GATE PERMEABILITY=RATIOK
C    COSTS COEFFICIENTS:
C       E1 = COST PER UNIT LENGTH OF FUNNEL WING WALL
C       E2 = COST PER UNIT LENGTH OF GATE LENGTH
C       E3 = COST PER UNIT GATE WIDTH
C       E11 = LAND COSTS PER UNIT AREA
C       E12 = COSTS PER UNIT VOLUME OF REACTIVE MEDIA
C
C THE SUBROUTINE RETURNS WITH FUNNEL/GATE DIMENSIONS AND COSTS
C STORED
C IN SEVERAL COMMON BLOCK ARRAYS INCLUDING:
C    GATEL(J)--AN ARRAY CONTAINING CALCULATED GATE LENGTHS (IN
C METERS)
C       FOR SYSTEM CONFIGURATION J
C    VOL(J)--AN ARRAY CONTAINING CALCULATED GATE VOLUMES (IN CUBIC
C METERS)
C       FOR SYSTEM CONFIGURATION J
C    WING(J)--AN ARRAY CONTAINING CALCULATED FUNNEL WALL LENGTHS (IN
C METERS)
C       FOR SYSTEM CONFIGURATION J
```

```
C     RL(J)--AN ARRAY CONTAINING CALCULATED PROJECTED FUNNEL WALL
C LENGTHS (IN METERS)
C        FOR SYSTEM CONFIGURATION J
C     TCOST(J)--AN ARRAY CONTAINING CALCULATED TOTAL SYSTEM COSTS
C        FOR SYSTEM CONFIGURATION J
C
C FINALLY THE SUBROUTINE HYD RETURNS WITH A VALUE FOR K, AN INTEGER
C VARIABLE THAT RECORDS
C WHICH OF THE SEVERAL SYSTEM CONFIGURATIONS EXAMINED, PRODUCED
C THE LOWEST CALCULATED
C TOTAL COST. THUS, BY LETTING J=K IN THE ABOVE ARRAYS, WE IDENTIFY THE
C DIMENSIONS OF A SYSTEM
C THAT IS A GOOD FIRST ESTIMATE OF THE MINIMUM COST CONFIGURATION.
C THESE DIMENSIONS ARE
C USED LATER AS INITIAL DECISION VARIABLE ESTIMATE IN SUBROUTINE OPTI,
C A NONLINEAR
C OPTIMIZATION ROUTINE DESIGNED TO IDENTIFY THE TRUE MINIMUM COST
CONFIGURATION.
C
      SUBROUTINE HYD(X,BR,GATEL,VOL,WING,RL,RATIOK,RKP,RPHI1,Q,BIGB
     /,TCOST,THETA,E1,E2,E3,E11,E12,K)
      IMPLICIT DOUBLE PRECISION (A-H, O-Z)
      DIMENSION BR(10),GATEL(10),VOL(10),WING(10),RL(10),
     /TCOST(10),ANGLE(10)
      CHARACTER*6 ATM1,ATM2,ATM3
      CHARACTER*7 ATM4,ATM5,ATM7,ATM8,ATM11,ATM12,ATM19
      CHARACTER*9 ATM9
      CHARACTER*13 ATM10
      CHARACTER*11 ATM13,ATM14
      CHARACTER*12 ATM6
C
C FOR VARIOUS b/B RATIOS DETERMINE THE LENGTH OF THE
C REACTOR ZONE "l" AND THE PROJECTED FUNNEL WALL LENGTH, "L"
C (SEE REPORT FOR DEFINITIONSC OF "L" AND "l")
C
C
C OUTPUT HEADER
      ATM1 = ' WIDTH'
      ATM2 = 'LENGTH'
      ATM3 = 'VOLUME'
      ATM4 = '[ M^3 ]'
      ATM5 = ' [ M ] '
      ATM6 = 'THOUSANDS OF'
```

```
      ATM7 = ' GATE '
      ATM8 = ' FUNNEL'
      ATM9 = 'PROJECTED'
      ATM10 = 'DIMENSIONLESS'
      ATM14 = ' PARAMETERS'
      ATM11= '  b/B  '
      ATM12 = '  L/l  '
      ATM13 = 'TOTAL COSTS'
      ATM19 = 'DOLLARS'
C
      WRITE(12,*)" "
      WRITE(12,72) ATM7,ATM8,ATM10,ATM13
 72   FORMAT(10X,A7,16X,A7,11X,A13,5X,A11)
      WRITE(12,74) ATM14
 74   FORMAT(52X,A11)
      WRITE(12,73) ATM1,ATM2,ATM3,ATM2,ATM9,ATM11,ATM12
 73   FORMAT(1X,A6,3X,A6,3X,A6,4X,A6,3X,A9,2X,A7,3X,A7)
      WRITE(12,75) ATM2,ATM6
 75   FORMAT(40X,A6,23X,A12)
      WRITE(12,76)ATM5,ATM5,ATM4,ATM5,ATM5,ATM19
 76   FORMAT(1X,A7,2X,A7,1X,A7,4X,A7,4X,A7,24X,A7)
      WRITE(12,*)
C
C INITIAL VALUE OF RLOLD = 0. AND K = 0 WHERE K IS DEFINED ABOVE AND
C RLOLD
C STORES CALCULATED VALUES OF THE PROJECTED FUNNEL LENGTHS
C BETWEEN SUCCESSIVE INTERATIONS USED TO OBTAIN A CONVERGENT
C SOLUTION TO
C PROJECTED FUNNEL WALL LENGTH RL(J) FOR THE SPECIFIC b/B RATIO OR BR(J)
OF INTEREST.
C
      RLOLD = 0.
      K=0
C
C THE BEGINNING OF A LOOP THAT CYCLES THOUGH 10 POTENTIAL VALUES OF
C THE
C b/B RATIO TO CALCULATED 10 POTENTIAL FUNNEL/GATE CONFIGURATIONS
C
      DO 90 I=1,10
C
C TCOST 'TOTAL COST AN INITIALLY LARGE VALUE SO THAT THE CHECK IF
C STATEMENT BEFORE
C THE CONTINUE STATEMENT SEES A DECREASING COST AND DOES NOT
```

```
C PREMATURELY ASSIGN K
C AN INCORRECT VALUE
C
      TCOST(I) = 1000000000000.
C
C RATIOB HOLD THE CURRENT VALUE OF b/B BEING USED TO CONFIGURE A
C SYSTEM
      RATIOB = BR(I)
C
C FROM CHRISTENSEN AND HATFIELD (1994) IT IS PREFERABLE TO NOT
C EXAMINE SYSTEM CONFIGURATIONS WITH b/B RATIOS LESS THAN OR EQUAL
C TO k/ko = RATIOK
      IF(BR(I).LE.RATIOK) GO TO 90
C
C THE FOLLOWING CLUSTER OF 5 LINES GIVE AN INITIAL CALCULATION OF THE
C PROJECTED
C LENGTH OF THE FUNNEL OR WING WALL RL(I).  NOTE: THE DURING THIS
C INITIAL CALCULATION
C TERM3, WHICH IS EQUAL TO THE SATURATED THICKNESS OF THE AQUIFER AT
C THE GATE ENTRANCE,
C IS APPROXIMATED WITH RPHI1, THE SATURATED AQUIFER THICKNESS AT THE
C UPGRADIENT ENTRANCE
C OF THE FUNNEL
      TERM3 = RPHI1
      TERM1 = 0.5*((RATIOK/RATIOB)-1.)
      TERM2 = DLOG(RATIOB)/(1.- RATIOB) + 1.
      TERM4 = Q*X/(THETA*BIGB*RATIOB)
 50   RL(I) = TERM1*TERM4/(TERM3*TERM2)
C
C AFTER THE FIRST INTERATION, TERM3 IS NOW CALCULATED USING A
C PREVIOUSLY CALCULATED RL(I)
C AS DEFINED BY EQUATION ***** IN THE REPORT
C
      TERM3 = (RPHI1*RPHI1 + 2.0*RL(I)*Q*DLOG(RATIOB)/
     /(RKP*BIGB*(1.0-RATIOB)))**0.5
C
C ABSOLUTE RELATIVE DEFERENCE BETWEEN SUCCESSIVE CALCULATIONS OF
C RL(I) ARE EXPRESSED WITH THE
C VARIABLE 'ERROR' WHERE RLOLD CONTAINES THE CALCULATED VALUE OF
C RL(I) FROM THE PREVIOUS
C ITERATION
C
      ERROR = ABS((RL(I)-RLOLD)/RL(I))
```

```
      RLOLD = RL(I)
C IF THE DIFFERENCE BETWEEN RL(I) VALUES CALCULATED BETWEEN
C INTERATIONS IS GREATER THAN 1 PERCENT
C THE PROGRAM RETURNS TO LINE 50 AND RECALCULATES RL(I)
      IF(ERROR.GT..01) GO TO 50
C
C
C CALCULATED A GATE LENGTH = GATEL(I)
C
      GATEL(I) = RL(I)*TERM2/TERM1
C
C CHECK RESIDENCE TIME, X IN THE REACTOR, HERE THE RESIDENCE TIME IS
C RECALCULATED TO COMPARE
C WITH THE INITIALLY SPECIFIED VALUE
C
      TERM4 = Q/(THETA*BIGB*RATIOB)
      TERM3 = (RPHI1*RPHI1 + 2.0*RL(I)*Q*DLOG(RATIOB)/
     /(RKP*BIGB*(1.0-RATIOB)))**0.5
      X = GATEL(I)*TERM3/TERM4
C
C CALCULATE GATE VOLUME
C
      VOL(I) = GATEL(I)*RATIOB*BIGB*TERM3
C
C CALCULATE LENGTH OF WING WALL
C
      TERM = (BIGB*BIGB*(1.- RATIOB)**2.0)/4.0
      WING(I) = (RL(I)*RL(I) + TERM)**0.5
C
C CALCULATE ANGLE OF WING WALL
C
      ANGLE(I) = ASIN(BIGB*(1.-RATIOB)/(2.*WING(I)))
C
C CALCULATE TOTAL FUNNEL/GATE COST
C
      TCOST(I)=4.*E1*WING(I)+2.*(GATEL(I)*E2 + E3*BIGB*RATIOB)
     /+E11*BIGB*(GATEL(I)+2.*RL(I))+E12*VOL(I)
C
C OUTPUT STATMENTS AS NEEDED TO CREATE A TABLE THAT SHOWS FOR
C SEVERAL VALUES
C OF THE b/B RATIO, DIMENSIONS OF ASSOCIATED FUNNEL/GATE SYSTEM AND
C  THEIR TOTAL COST
C
```

```
      WRITE(12,71)RATIOB*BIGB,GATEL(I),VOL(I),WING(I),RL(I),RATIOB,
     /RL(I)/GATEL(I),TCOST(I)
  71  FORMAT(1X,F6.2,2X,F6.2,4X,F6.2,2X,2X,F6.2,4X,F6.2,2X,F7.2,4X,F7.2
     /,2X,F10.0)
C
C THE FOLLOWING CONDITIONAL STATEMENT DETERMINES AT WHICH
C  ITERATION, I, A DESIGN
C CONFIGURATION WAS FOUND IN WHICH THE TOTAL COST INCREASED FROM
C THE PREVIOUS
C ITERATION; THUS, DEFINING THE ITERATION K = I-1, WHERE A SPECIFIED b/B
C  RATIO PRODUCED
C THE LOWEST COST SYSTEM CONFIGURATION.
      IF(I.GT.1.AND.TCOST(I).GT.TCOST(I-1).AND.K.EQ.0)K=I-1
  90  CONTINUE
C
C SUBROUTINE HAS COMPLETED CALCULATIONS FOR A SUITE OF SYSTEMS
C DEFINED BY THE CRITICAL HYDRAULIC
C RESIDENCE TIME,X AND THE b/B RATIO.
      RETURN
      END
```

Subroutine OPTI.for:

```
C SUBROUTINE OPTI CONTAINS APPROPRIATE RELATIONSHIPS THE MINIMUM
C COST
C FUNNEL/GATE DESIGN CONFIGURATIONS THAT PRODUCE SUFFICIENT
C HYDRAULIC RESIDENCE TIME, TD, WITHIN THE REACTIVE GATE.
C
C PARAMETERS USED BY THE SUBROUTINE INCLUDE:
C    THE PLUME WIDTH=BIGB,IN METERS
C    THE MINIMUM REQUIRED HYDRAULIC DETENTION TIME, X, IN DAYS,
C PROVIDED BY
C       SUBROUTINE TRANS
C    THE AQUIFER DISCHARGE=Q (IN CUBIC METERS/DAY), ACROSS THE PLUME
C WIDTH
C    THE POROSITY OF THE GATE = THETA
C    SATURATED THICKNESS=RPHI1, IN METERS
C    THE PERMEABILITY OF THE AQUIFER=RKP, IN METERS/DAY
C    THE RATIO OF AQUIFER TO GATE PERMEABILITY=RATIOK
C    AN INITIAL ESTIMATE OF THE GATE WIDTH TO FUNNEL WIDTH RATIO, b/B, =
C X1,
C       GENERATED BY SUBROUTINE HYD AND TRANSFERRED THROUGH
C VARIABLE XX1
C    AN INITIAL ESTIMATE OF THE FUNNEL WALL LENGTH (IN METERS), = X2,
C       GENERATED BY SUBROUTINE HYD AND TRANSFERRED THROUGH
C VARIABLE XX2
C    AN INITIAL ESTIMATE OF THE GATE LENGTH (IN METERS),= X3,
C       GENERATED BY SUBROUTINE HYD AND TRANSFERRED THROUGH
C VARIABLE XX3
C    AN INITIAL ESTIMATE OF THE PROJECTED FUNNEL WALL LENGTHS (IN
C METERS), = X4,
C       GENERATED BY SUBROUTINE HYD AND TRANSFERRED THROUGH
C VARIABLE XX4
C    COSTS COEFFICIENTS:
C       E1 = COST PER UNIT LENGTH OF FUNNEL WING WALL
C       E2 = COST PER UNIT LENGTH OF GATE LENGTH
C       E3 = COST PER UNIT GATE WIDTH
C       E11 = LAND COSTS PER UNIT AREA
C       E12 = COSTS PER UNIT VOLUME OF REACTIVE MEDIA
C    INITIAL ESTIMATES OF LAGRANGIAN MULTIPLIERS X6,X7,X8, AND X9
C    DEPTH OF FUNNEL/GATE WALLS OR DEPTH TO AQUICLUDE, DEPTH
C
C THE SUBROUTINE FINDS THE DIMENSIONS OF THE MINIMUM COST
C FUNNEL/GATE CONFIGURATION
```

```
C THEN RECORDS THOSE DIMENSIONS (i.e., GATE LENGTH, FUNNEL WALL
C LENGTH,
C PROJECTED FUNNEL WALL LENGTH, GATE WIDTH TO PLUME WIDTH RATIO,
C AND THE SATURATED
C AQUIFER THICKNESS IN THE GATE) TO THE OUTPUT FILE.  FINALLY THE
C SUBROUTINE RECORDS
C THE TOTAL COST OF THE SYSTEM.
C
C
      SUBROUTINE OPTI(BIGB,X,Q,THETA,RPHI1,RKP,RATIOK,XX1,XX2,XX3,XX4,
     /E1,E2,E3,E11,E12,X6,X7,X8,X9,DEPTH)
      IMPLICIT DOUBLE PRECISION (A-H, O-Z)
      DIMENSION A(9,9),B(9,2),XX(4)
      COMMON A,B
      CHARACTER*6 ATM1,ATM2,ATM3
      CHARACTER*7 ATM4,ATM5,ATM7,ATM8,ATM11,ATM12,ATM19
      CHARACTER*9 ATM9
      CHARACTER*13 ATM10
      CHARACTER*12 ATM6
      CHARACTER*11 ATM13,ATM14
      CHARACTER*38 ATM15,ATM16,ATM17,ATM18
C
C
C
C OUTPUT HEADER
      ATM1 = ' WIDTH'
      ATM2 = 'LENGTH'
      ATM3 = 'VOLUME'
      ATM4 = '[ M^3 ]'
      ATM5 = ' [ M ] '
      ATM6 = 'THOUSANDS OF'
      ATM7 = ' GATE '
      ATM8 = ' FUNNEL'
      ATM9 = 'PROJECTED'
      ATM10 = 'DIMENSIONLESS'
      ATM14 = ' PARAMETERS'
      ATM11= ' b/B '
      ATM12 =' L/l '
      ATM13 = 'TOTAL COSTS'
      ATM15 = 'TOTAL FUNNEL/GATE WALL AREA [ M^2 ] = '
      ATM16 = 'TOTAL FUNNEL WALL AREA [ M^2 ]    = '
      ATM17 = 'TOTAL GATE LENGTH WALL AREA [ M^2 ] = '
      ATM18 = 'TOTAL GATE WIDTH WALL AREA [ M^2 ]  = '
```

```
      ATM19 = 'DOLLARS'
C

      WRITE(12,*)" "
      WRITE(12,*)" "
      WRITE(12,*)" "
      WRITE(12,*)" ********** MINIMUM COST DESIGN ********   "
      WRITE(12,*)" "
      WRITE(12,*)" "
      WRITE(12,72) ATM7,ATM8,ATM10,ATM13
 72   FORMAT(10X,A7,16X,A7,11X,A13,5X,A11)
      WRITE(12,74) ATM14
 74   FORMAT(52X,A11)
      WRITE(12,73) ATM1,ATM2,ATM3,ATM2,ATM9,ATM11,ATM12
 73   FORMAT(1X,A6,3X,A6,3X,A6,4X,A6,3X,A9,2X,A7,3X,A7)
      WRITE(12,75) ATM2,ATM6
 75   FORMAT(40X,A6,23X,A12)
      WRITE(12,76)ATM5,ATM5,ATM4,ATM5,ATM5,ATM19
 76   FORMAT(1X,A7,2X,A7,1X,A7,4X,A7,4X,A7,24X,A7)
      WRITE(12,*)
C
C
C PARAMETERS NP,MP,N,AND M ARE DIMINSIONS USED IN CONSTRUCTING
C ARRAYS USED
C IN SUBROUTINE GAUSSJ...A GAUSS-JORDAN SOLVER PRESENTED IN
C "NUMERICAL RECIPIES IN FORTRAN" BY PRESS et al. (1993)
C
C ONE NEED ONLY REMEMBER THAT NP=N WHICH IS THE NUMBER OF
C VARIABLES AND THE
C NUMBER OF EQUATIONS TO BE SOLVED AS GENERATED FROM FIRST
CREATING
C THE LAGRANGIAN
C AND THEN SUBSEQUENTLY DEFINING THE NECESSARY CONDITIONS FOR A
C STATIONARY POINT
C FOR THE LAGRANGAIN....AND M IS THE NUMBER OF KNOWN CONSTANTS
C DEFINING THE RIGHT-HAND-SIDE
C OF EACH EQUATION.
C
      NP=9
      MP=2
      N=9
      M=1
C
C PARAMETER DEFINITIONS AS SPECIFIED IN THE REPORT
```

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```
C
C       E4 = THE FUNNEL WIDTH "BIGB"
C
      E4 = BIGB
C
C       E5 = EQUIVALENT TO THE KNOWN PRODUCT OF GATE WIDTH 'b' FLOW
C THICKNESS,
C       RPHI, AND GATE LENGTH,l.
C
      E5=X*Q/THETA
C
      E7=RPHI1**2.
      E8=2.*Q/(RKP*BIGB)
      E9 = BIGB*BIGB/4.
      E10 = RATIOK
      XX(1) = X9
      XX(2) = 10.*X9
      XX(3) = 100.*X9
      XX(4) = 500.*X9
      DO 800 IK=1,4
C INITIAL VARIABLE ESTIMATES
      X1 = XX1
      X2 = XX2
      X3 = XX3
      X4 = XX4
      X5 = RPHI1
      X9=XX(IK)
C     PRINT*,X1,X2,X3,X4,X5
      ITER = 0
C ************************************************************
C THIS IS THE BEGINNING OF THE APPLICATION OF THE NEWTON-RAPHSON
C SOLUTION
C ALGORITHM
C
C DEFINING DELTA VALUES
      DX1 = 0.
      DX2 = 0.
      DX3 = 0.
      DX4= 0.
      DX5 = 0.
      DX6 = 0.
      DX7 = 0.
      DX8 = 0.
```

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```
      DX9 = 0.
C CALCULATE UPDATED PARAMETER ESTIMATES AND FUNCTIONS VALUES
1     ITER = 1 + ITER
      X1 = X1 + DX1
      X2 = X2 + DX2
      X3 = X3 + DX3
      X4 = X4 + DX4
      X5 = X5 + DX5
      X6 = X6 + DX6
      X7 = X7 + DX7
      X8 = X8 + DX8
      X9 = X9 + DX9
      TM1 = 2.*E3*E4 + X6*E4*X3*X5
      TM2 = X7*(-X5*X5 + E7 - E8*X4/X1)
      TM3 = - X8*E9*(-2. + 2.*X1)
      TM4 = X9*(2.*X4*(DLOG(X1) + 2. - 2.*X1))
      TM5 = X9*(-X3*(-E10 - 1. + 2.*X1))
      F1 = TM1+TM2+TM3+TM4+TM5
      F2 = 4.*E1 + X8*2.*X2
      TM1 = 2.*E2 + E11*E4 + X6*E4*X1*X5
      TM2 = - X9*(E10*(1.-X1) - X1 + X1*X1)
      F3 = TM1+TM2
      TM1 = 2.*E11*E4 - 2.*X8*X4
      TM2 = X9*2.*(X1*DLOG(X1) + X1 - X1*X1)
      F4 = TM1+TM2
      F5 = X6*E4*X1*X3 + X7*2.*X5*(1.- X1)
      F6 = E4*X1*X3*X5 - E5
      F7 = X5*X5*(1.-X1) - E7*(1.-X1) - E8*X4*DLOG(X1)
      F8 = X2*X2 - E9*(1.- 2.*X1 + X1*X1) - X4*X4
      TM1 = 2.*X4*(X1*DLOG(X1) + X1 - X1*X1)
      TM2 = - X3*(E10*(1.-X1) - X1 + X1*X1)
      F9 = TM1 + TM2
C DEFINING UPDATED MATRIX ELEMENTS TO BE USED IN THE GAUSSJ.FOR
C SUBROUTINE.
      B(1,1) = - F1
      B(2,1) = - F2
      B(3,1) = - F3
      B(4,1) = - F4
      B(5,1) = - F5
      B(6,1) = - F6
      B(7,1) = - F7
      B(8,1) = - F8
      B(9,1) = - F9
```

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```
C
C HERE WE ARE DEFINING THE ELEMENTS OF THE JACOBIAN MATRIX, THESE
C FUNCTION WERE DERIVED
C FROM THE DERIVATIVES OF F1,F2,F3,F4,F5,F6,F7,F8,AND F9  (EQS.4-24 THROUGH
C 4-32)
C TAKEN WITH RESPECT TO THE NINE VARIABLES
C
      TM1 = X7*E8*X4/(X1*X1) - X8*E9*2.
      TM2 = X9*(2.*X4/X1 - 4.*X4 - 2.*X3)
      A(1,1) = TM1+TM2
      A(1,2) = 0.
      A(1,3) = X6*E4*X5 - X9*(-E10 - 1. + 2.*X1)
      A(1,4) = -X7*E8/X1 + 2.*X9*(DLOG(X1) + 2. - 2.*X1)
      A(1,5) = X6*E4*X3 - 2.*X7*X5
      A(1,6) = E4*X3*X5
      A(1,7) = - X5*X5 + E7 - E8*X4/X1
      A(1,8) = - E9*(-2.+2.*X1)
      TM1 = 2.*X4*(DLOG(X1) + 2. - 2.*X1)
      TM2 = - X3*(-E10 - 1. + 2.*X1)
      A(1,9) = TM1 + TM2
      A(2,1) = 0.
      A(2,2) = 2.*X8
      A(2,3) = 0.
      A(2,4) = 0.
      A(2,5) = 0
      A(2,6) = 0.
      A(2,7) = 0.
      A(2,8) = 2.*X2
      A(2,9) = 0.
      A(3,1) = X6*E4*X5 - X9*(-E10 - 1. + 2.*X1)
      A(3,2) = 0.
      A(3,3) = 0.
      A(3,4) = 0.
      A(3,5) = X6*E4*X1
      A(3,6) = E4*X1*X5
      A(3,7) = 0.
      A(3,8) = 0.
      A(3,9) = - E10*(1.-X1) + X1 - X1*X1
      A(4,1) = X9*2.*(DLOG(X1) + 2. - 2.*X1)
      A(4,2) = 0.
      A(4,3) = 0.
      A(4,4) = -2.*X8
      A(4,5) = 0.
```

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```
A(4,6) = 0.
A(4,7) = 0.
A(4,8) = - 2.*X4
A(4,9) = 2.*(X1*DLOG(X1) + X1 - X1*X1)
A(5,1) = X6*E4*X3 - X7*2.*X5
A(5,2) = 0.
A(5,3) = X6*E4*X1
A(5,4) = 0.
A(5,5) = 2.*X7*(1.-X1)
A(5,6) = E4*X1*X3
A(5,7) = 2.*X5*(1.-X1)
A(5,8) = 0.
A(5,9) = 0.
A(6,1) = E4*X3*X5
A(6,2) = 0.
A(6,3) = E4*X1*X5
A(6,4) = 0.
A(6,5) = E4*X1*X3
A(6,6) = 0.
A(6,7) = 0.
A(6,8) = 0.
A(6,9) = 0.
A(7,1) = - X5*X5 + E7 - E8*X4/X1
A(7,2) = 0.
A(7,3) = 0.
A(7,4) = - E8*DLOG(X1)
A(7,5) = 2.*X5*(1.-X1)
A(7,6) = 0.
A(7,7) = 0.
A(7,8) = 0.
A(7,9) = 0.
A(8,1) = - E9*(-2. + 2.*X1)
A(8,2) = 2.*X2
A(8,3) = 0.
A(8,4) = -2.*X4
A(8,5) = 0.
A(8,6) = 0.
A(8,7) = 0.
A(8,8) = 0.
A(8,9) = 0.
A(9,1) = 2.*X4*(DLOG(X1) + 2. - 2.*X1) - X3*(-E10 - 1.+ 2.*X1)
A(9,2) = 0.
A(9,3) =- E10*(1.- X1) + X1 - X1*X1
```

```fortran
      A(9,4) = 2.*(X1*DLOG(X1) + X1 - X1*X1)
      A(9,5) = 0.
      A(9,6) = 0.
      A(9,7) = 0.
      A(9,8) = 0.
      A(9,9) = 0.
C
C NOW WE CALL GAUSSJ BECAUSE WE WILL BE
C SOLVING FOR THE UPDATE DELTA VALUES (WHICH WILL BRING US CLOSER TO
C THE LOWEST COST DESIGN
C
      CALL GAUSSJ(A,N,NP,B,M,MP)
      DX1 = B(1,1)
      DX2 = B(2,1)
      DX3 = B(3,1)
      DX4 = B(4,1)
      DX5 = B(5,1)
      DX6 = B(6,1)
      DX7 = B(7,1)
      DX8 = B(8,1)
      DX9 = B(9,1)
C
C CHECK TO SEE IF VARIABLE X1 IS APPROACHING A VALUE OF 1...IF SO WE
C CHOOSE A NEW
C INITIAL VALUE FOR LAGRANGIAN VARIABLE X9
C
      IF(X1.GT..95) GO TO 800
C CHECK RELATIVE CHANGES IN PARAMETER ESTIMATES BETWEEN
C INTERATIONS
      IF(DX1.LT..000000001) GO TO 300
      IF(ABS(DX1/X1).GE..005) GO TO 1
  300 IF(DX2.LT..000000001) GO TO 301
      IF(ABS(DX2/X2).GE..005) GO TO 1
  301 IF(DX3.LT..000000001) GO TO 302
      IF(ABS(DX3/X3).GE..005) GO TO 1
  302 IF(DX4.LT..000000001) GO TO 303
      IF(ABS(DX4/X4).GE..005) GO TO 1
  303 IF(DX5.LT..000000001) GO TO 304
      IF(ABS(DX5/X5).GE..005) GO TO 1
  304 IF(DX6.LT..000000001) GO TO 305
      IF(ABS(DX6/X6).GE..005) GO TO 1
  305 IF(DX7.LT..000000001) GO TO 306
      IF(ABS(DX7/X7).GE..005) GO TO 1
```

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```
306  IF(DX8.LT..000000001) GO TO 307
     IF(ABS(DX8/X8).GE..005) GO TO 1
307  IF(DX9.LT..000000001) GO TO 312
     IF(ABS(DX9/X9).GE..005) GO TO 1
     GO TO 312
C PRINT FINAL OPTIMUM PARAMETER ESTIMATES
800  CONTINUE
C 312  PRINT*,X1,X2,X3,X4,X5
C     PRINT*,X6,X7,X8,X9,ITER
312  TCOST = 4.*E1*X2 +2.*E2*X3 + 2.*E3*E4*X1 + E11*E4*(X3+2.*X4)
    /+ E12*E5
C     TAREA = TOTAL FUNNEL/GATE WALL AREA [ M^2 ]
C     TFWA = TOTAL FUNNEL WALL AREA [ M^2 ]
C     TGLA = TOTAL GATE LENGTH WALL AREA [ M^2 ]
C     TGWA = TOTAL GATE WIDTH WALL AREA [ M^2 ]
     TAREA = 4.*DEPTH*X2 +2.*DEPTH*X3 + 2.*DEPTH*BIGB*X1
     TFWA = 4.*DEPTH*X2
     TGLA = 2.*DEPTH*X3
     TGWA = 2.*DEPTH*BIGB*X1
     WRITE(6,*)" ********** MINIMUM COST DESIGN ********  "
     WRITE(6,*)" "
     WRITE(6,*)" "
     WRITE(6,72) ATM7,ATM8,ATM10,ATM13
     WRITE(6,74) ATM14
     WRITE(6,73) ATM1,ATM2,ATM3,ATM2,ATM9,ATM11,ATM12
     WRITE(6,75) ATM2,ATM6
     WRITE(6,76)ATM5,ATM5,ATM4,ATM5,ATM5,ATM19
     WRITE(6,*)" "
     WRITE(6,71)X1*BIGB,X3,X1*BIGB*X5*X3,X2,X4,X1,X4/X3,TCOST
     WRITE(6,*)" "
     WRITE(6,*)" "
     WRITE(6,*)" "
     WRITE(6,78)ATM15,TAREA
     WRITE(6,*)" "
     WRITE(6,*)" "
     WRITE(6,*)" "
78   FORMAT(2X,A38,F6.1)
     WRITE(12,71)X1*BIGB,X3,X1*BIGB*X5*X3,X2,X4,X1,X4/X3,TCOST
71   FORMAT(1X,F6.2,2X,F6.2,4X,F6.2,2X,2X,F6.2,4X,F6.2,2X,F7.2,4X,F7.2
    /,2X,F10.0)
     WRITE(12,*)" "
     WRITE(12,*)" "
     WRITE(12,*)" "
```

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```
WRITE(12,78)ATM16,TFWA
WRITE(12,78)ATM18,TGWA
WRITE(12,78)ATM17,TGLA
WRITE(12,78)ATM15,TAREA
RETURN
END
```

Subroutine GAUSSJ.for:

```fortran
      SUBROUTINE GAUSSJ(A,N,NP,B,M,MP)
      PARAMETER (NMAX=50)
      IMPLICIT DOUBLE PRECISION (A-H, O-Z)
      DIMENSION A(NP,NP),B(NP,MP),IPIV(NMAX),INDXR(NMAX),INDXC(NMAX)
      DO 11 J=1,N
        IPIV(J)=0
11    CONTINUE
      DO 22 I=1,N
        BIG=0.
        DO 13 J=1,N
          IF(IPIV(J).NE.1)THEN
            DO 12 K=1,N
              IF(IPIV(K).EQ.0) THEN
                IF(ABS(A(J,K)).GE.BIG) THEN
                BIG=ABS(A(J,K))
                IROW=J
                ICOL=K
                ENDIF
              ELSE IF (IPIV(K).GT.1) THEN
                PAUSE 'SINGULAR MATRIX'
              ENDIF
12          CONTINUE
          ENDIF
13      CONTINUE
        IPIV(ICOL)=IPIV(ICOL)+1
        IF(IROW.NE.ICOL) THEN
          DO 14 L=1,N
            DUM=A(IROW,L)
            A(IROW,L)=A(ICOL,L)
            A(ICOL,L)=DUM
14        CONTINUE
          DO 15 L=1,M
            DUM=B(IROW,L)
            B(IROW,L)=B(ICOL,L)
            B(ICOL,L)=DUM
15        CONTINUE
        ENDIF
        INDXR(I)=IROW
        INDXC(I)=ICOL
        IF (A(ICOL,ICOL).EQ.0.) PAUSE 'SINGULAR MARTRIX'
        PIVINV=1./A(ICOL,ICOL)
```

```fortran
      A(ICOL,ICOL)=1.
      DO 16 L=1,N
        A(ICOL,L)=A(ICOL,L)*PIVINV
16      CONTINUE
      DO 17 L=1,M
        B(ICOL,L)=B(ICOL,L)*PIVINV
17      CONTINUE
    DO 21 LL=1,N
      IF(LL.NE.ICOL)THEN
        DUM=A(LL,ICOL)
        A(LL,ICOL)=0.
        DO 18 L=1,N
          A(LL,L)=A(LL,L)-A(ICOL,L)*DUM
18        CONTINUE
        DO 19 L=1,M
          B(LL,L)=B(LL,L)-B(ICOL,L)*DUM
19          CONTINUE
      ENDIF
21      CONTINUE
22    CONTINUE
    DO 24 L=N,1,-1
      IF(INDXR(L).NE.INDXC(L)) THEN
        DO 23 K=1,N
          DUM=A(K,INDXR(L))
          A(K,INDXR(L))=A(K,INDXC(L))
          A(K,INDXC(L))=DUM
23        CONTINUE
      ENDIF
24    CONTINUE
    RETURN
    END
```

Example Input File:

STD1 [ug/l] STD2 [ug/l] STD3 [ug/l] STD4 [ug/l] DT(TIMESTEP) [DAYS]
*
 5.0   5.0   70.0   1.0   .1
*
FUNNEL WIDTH [M] GRADIENT AQU. THICKNESS [M] AQU. HYDRAULIC COND. [M/d]
*
 61.   -0.005   5.   4.32
*
GATE POROSITY HYDRAULIC COND. RATIO (AQUIFER/GATE) DEPTH OF SYSTEM WALLS [M]
*
 .45   .1   6.
*
VARIOUS RATIOS OF GATE WIDTH TO PLUME WIDTH b/B EXAMINED
*
BR(1) BR(2) BR(3) BR(4) BR(5)
*
.02   .05   .1   .2   .4
*
BR(6) BR(7) BR(8) BR(9) BR(10)
*
.5   .6   .7   .8   .9
*
****DATA PLUME CONTAMINANT CONCENTRATIONS AND DEGRADATION PARAMETERS
*
PLUME C1 CONC. [ug/l] LAMBDA 1A [1/DAY] LAMBDA 1B [1/DAY]
*
 5000.   36.9   0.
*
PLUME C2 CONC. [ug/l] LAMBDA 2A [1/DAY] LAMBDA 2B [1/DAY]
*
  5000.   3.69   33.18
*
PLUME C3 CONC. [ug/l] LAMBDA 3A [1/DAY] LAMBDA 3B [1/DAY]
*
   0.   .8318   0.
*
PLUME C4 CONC. [ug/l] LAMBDA 4A [1/DAY]

```
*
       0.              .8318
*
* READ IN COSTS COEFFICIENTS: [ IN UNITS OF THOUSANDS OF DOLLARS ]
*      CSFFW = COST PER UNIT AREA OF FUNNEL WALL MATERIAL
*      CSFGL = COST PER UNIT AREA OF LONGITUDINAL GATE WALL
*      CSFGW = COST PER UNIT AREA OF TRANSVERSE GATE WALL
*      E11 = LAND COSTS PER UNIT AREA
*      E12 = REACTIVE MEDIA COSTS PER UNIT VOLUME
*

  CSFFW    CSFGL     CSFGW      E11     E12
*

   .193     .193    .193     .001    1.725
*

* READ IN INITIAL ESTIMATES OF LAGRANGIAN MULTIPLIERS, X6, X7, X8, AND X9
*

X6    X7    X8      X9
*

1.    1.    1.     10.
```

Example Output File:

TIME	C1	C2	C3	C4
[DAY]	[ug/l]	[ug/l]	[ug/l]	[ug/l]
.00	5000.00	5000.00	.00	.00
.10	124.86	586.66	879.91	48.15
.20	3.12	26.22	873.98	115.50
.30	.08	.94	806.89	173.34
.40	.00	.03	742.58	221.27
.50	.00	.00	683.31	260.45
.60	.00	.00	628.77	291.96
.70	.00	.00	578.59	316.79
.80	.00	.00	532.41	335.79
.90	.00	.00	489.91	349.74
1.00	.00	.00	450.81	359.32
1.10	.00	.00	414.83	365.15
1.20	.00	.00	381.72	367.76
1.30	.00	.00	351.25	367.62
1.40	.00	.00	323.22	365.16
1.50	.00	.00	297.42	360.76
1.60	.00	.00	273.68	354.73
1.70	.00	.00	251.84	347.36
1.80	.00	.00	231.74	338.92
1.90	.00	.00	213.24	329.60
2.00	.00	.00	196.22	319.62
2.10	.00	.00	180.56	309.13
2.20	.00	.00	166.15	298.27
2.30	.00	.00	152.89	287.18
2.40	.00	.00	140.68	275.96
2.50	.00	.00	129.46	264.71
2.60	.00	.00	119.12	253.49
2.70	.00	.00	109.62	242.37
2.80	.00	.00	100.87	231.42
2.90	.00	.00	92.82	220.67
3.00	.00	.00	85.41	210.16
3.10	.00	.00	78.59	199.92
3.20	.00	.00	72.32	189.98
3.30	.00	.00	66.55	180.35
3.40	.00	.00	61.23	171.05
3.50	.00	.00	56.35	162.09

3.60	.00	.00	51.85	153.46
3.70	.00	.00	47.71	145.18
3.80	.00	.00	43.90	137.25
3.90	.00	.00	40.40	129.65
4.00	.00	.00	37.17	122.40
4.10	.00	.00	34.21	115.47
4.20	.00	.00	31.48	108.88
4.30	.00	.00	28.97	102.59
4.40	.00	.00	26.65	96.62
4.50	.00	.00	24.53	90.95
4.60	.00	.00	22.57	85.57
4.70	.00	.00	20.77	80.47
4.80	.00	.00	19.11	75.63
4.90	.00	.00	17.58	71.06
5.00	.00	.00	16.18	66.73
5.10	.00	.00	14.89	62.65
5.20	.00	.00	13.70	58.79
5.30	.00	.00	12.61	55.14
5.40	.00	.00	11.60	51.71
5.50	.00	.00	10.68	48.47
5.60	.00	.00	9.82	45.42
5.70	.00	.00	9.04	42.54
5.80	.00	.00	8.32	39.84
5.90	.00	.00	7.65	37.30
6.00	.00	.00	7.04	34.91
6.10	.00	.00	6.48	32.66
6.20	.00	.00	5.96	30.55
6.30	.00	.00	5.49	28.57
6.40	.00	.00	5.05	26.71
6.50	.00	.00	4.65	24.96
6.60	.00	.00	4.28	23.32
6.70	.00	.00	3.93	21.79
6.80	.00	.00	3.62	20.35
6.90	.00	.00	3.33	19.00
7.00	.00	.00	3.07	17.74
7.10	.00	.00	2.82	16.56
7.20	.00	.00	2.60	15.46
7.30	.00	.00	2.39	14.42
7.40	.00	.00	2.20	13.45
7.50	.00	.00	2.02	12.55
7.60	.00	.00	1.86	11.70
7.70	.00	.00	1.71	10.91
7.80	.00	.00	1.58	10.17

7.90	.00	.00	1.45	9.48
8.00	.00	.00	1.33	8.83
8.10	.00	.00	1.23	8.23
8.20	.00	.00	1.13	7.67
8.30	.00	.00	1.04	7.14
8.40	.00	.00	.96	6.65
8.50	.00	.00	.88	6.19
8.60	.00	.00	.81	5.77
8.70	.00	.00	.75	5.37
8.80	.00	.00	.69	5.00
8.90	.00	.00	.63	4.65
9.00	.00	.00	.58	4.33
9.10	.00	.00	.53	4.03
9.20	.00	.00	.49	3.75
9.30	.00	.00	.45	3.48
9.40	.00	.00	.42	3.24
9.50	.00	.00	.38	3.01
9.60	.00	.00	.35	2.80
9.70	.00	.00	.32	2.61
9.80	.00	.00	.30	2.42
9.90	.00	.00	.27	2.25
10.00	.00	.00	.25	2.09
10.10	.00	.00	.23	1.95
10.20	.00	.00	.21	1.81
10.30	.00	.00	.20	1.68
10.40	.00	.00	.18	1.56
10.50	.00	.00	.17	1.45
10.60	.00	.00	.15	1.35
10.70	.00	.00	.14	1.25
10.80	.00	.00	.13	1.16
10.90	.00	.00	.12	1.08
11.00	.00	.00	.11	1.00
11.10	.00	.00	.10	.93

CRITICAL HYDRAULIC RESIDENCE TIME =   11.10 [DAY]

GATE			FUNNEL		DIMENSIONLESS PARAMETERS		TOTAL COSTS
WIDTH	LENGTH	VOLUME	LENGTH	PROJECTED LENGTH	b/B	L/l	
[M]	[M]	[M^3]	[M]	[M]			THOUSANDS OF DOLLARS
12.20	2.67	162.50	24.41	.66	.20	.25	428.
24.40	1.33	162.50	18.32	.95	.40	.71	425.
30.50	1.07	162.50	15.29	1.11	.50	1.04	424.
36.60	.89	162.50	12.27	1.34	.60	1.50	424.
42.70	.76	162.50	9.31	1.73	.70	2.27	424.
48.80	.67	162.50	6.60	2.53	.80	3.78	426.
54.90	.60	162.50	5.80	4.93	.90	8.29	436.

********** MINIMUM COST DESIGN ********

GATE			FUNNEL		DIMENSIONLESS PARAMETERS		TOTAL COSTS
WIDTH	LENGTH	VOLUME	LENGTH	PROJECTED LENGTH	b/B	L/l	
[M]	[M]	[M^3]	[M]	[M]			THOUSANDS OF DOLLARS
36.60	.89	162.78	12.27	1.34	.60	1.50	424.

TOTAL FUNNEL WALL AREA [M^2]   = 294.6
TOTAL GATE WIDTH WALL AREA [M^2] = 439.2
TOTAL GATE LENGTH WALL AREA [M^2] = 10.7
TOTAL FUNNEL/GATE WALL AREA [M^2] = 744.4

SECTION VII

CONCLUSIONS

A series of equations which constitute an analytical, multi-contaminant, degradation and transport model have been developed. This model can be applied in iterative manner to determine the critical hydraulic residence time, T, required to achieve specified concentrations of contaminants within a gate (e.g., to be certain that the water quality at the gate exit meets a specified water quality standard i.e., 1 μg/l vinyl chloride). To use this transport model, the following data are needed:

a)   degradation rate coefficients for all reactions depicted in Figure 3;

b)   specified water quality goals or system performance standards for C_1, C_2, C_3, and C4 (e.g., primary drinking water standards for PCE, TCE, DCE, and vinyl chloride); and

c)   the concentration of each contaminant at the entrance of the gate, C_{10}, C_{20}, C_{30}, and C_{40}. Once the critical hydraulic residence time is known, the hydraulic model can be used to dimension the system.

From an existing analytical hydraulic model for funnel/gate systems developed by Christensen and Hatfield (1994), an iterative design algorithm was developed for dimensioning a funnel/gate system. The design algorithm requires the following site and system data to execute:

a)   the critical hydraulic residence time in the gate;

b)   the transverse width of groundwater flow to be intercepted within the funnel, B;

c)   the saturated thickness of the phreatic aquifer, ϕ_1, at the entrance of the funnel;

d)   the groundwater flow through the area defined by width B and flow thickness, ϕ_1;

e)   the aquifer hydraulic conductivity;

f)   the porosity of the reactive porous media within the gate; and

g)   the hydraulic conductivity of the porous media within the gate.

Results of two FRAC-3D numerical validation studies were also presented. For the two funnel/gate systems examined, the numerical results showed the analytical design model produced system configurations which exhibited 80 to 85 percent capture efficiency. These

efficiencies increase as the gate becomes wider. Thus, results of the numerical validation suggest the funnel/gate design model could be used to pre-dimension a system; however, subsequent numerical simulations should be conducted to verify the hydraulics of the design.

A funnel/gate cost estimation model was also developed to identify minimum cost designs subject to four constraints: one that defines the desired hydraulic retention time in the gate, one that defines the funnel wall length in terms of other system dimensions, and two that serve as hydraulic constraints. Costs considered in the model include land costs, costs per unit length of funnel walls, costs per unit length of gate, costs per unit width of gate, and costs associated with the reactive medium used in the gate.

The general cost model was recast into a Lagrangian optimization model. As a result of this reformulation, the optimization problem was reduced to that of solving a system of nine nonlinear equations with nine unknowns. Recommendations were given as to how the nine equations could be solved.

Finally a computer program was developed to demonstrate the theory that was developed. The Funnel/Gate Design Model (FGDM) software is a FORTRAN program developed to ascertain feasible dimensions of funnel/gate systems and also identify the lowest cost design. Feasible is defined here to include designs that are consistent with the transport and hydraulic theories outlined in Sections 2 and 3. Examples of input data and computational results are presented.

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